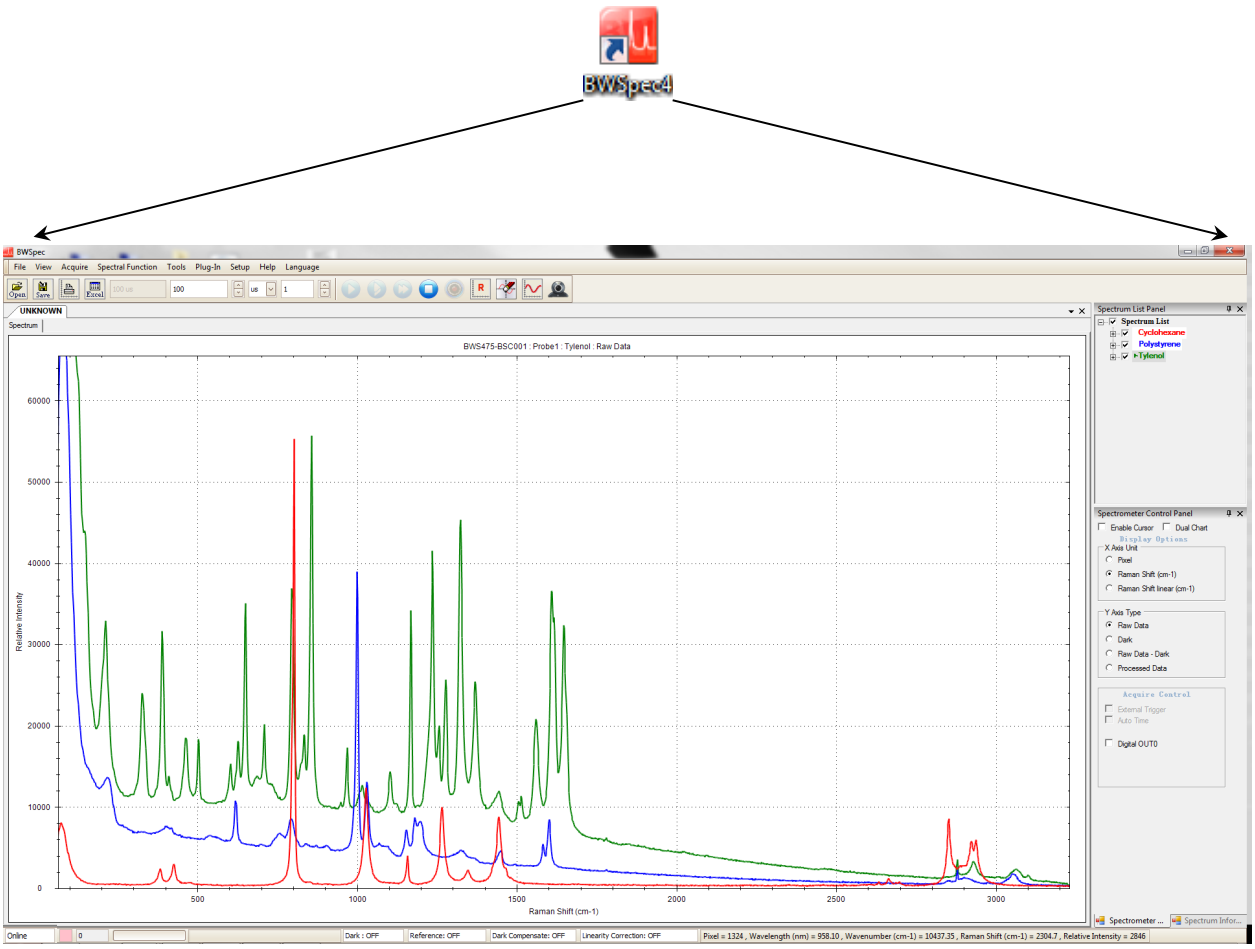
313 Enterprise Dr, Plainsboro, NJ 08536, USA
www.bwtek.com
+1.855.MY.BWTEK



BWSpec® 4.15 Software User Manual

Table of Contents

1 INTRODUCTION

BWSpec® 4 is a Spectrometer Data Acquisition and Analysis Software Program. It supports three types of B&W Tek spectrometer interfaces: RS-232, USB 2.0, and USB 3.0.

2 INSTALLATION

Refer to "BWSpec Software and Hardware Installation Guide" for fully detailed installation instructions: You may consult IT department for support.

Operation system

Windows 10 (32 bit & 64 bit)
Windows 11 64 bit
Administrator Windows user privilege for installation

*Hardware Requirements**

Meets or exceeds the System Requirements for your PC's Operating System respectively
Processor: 1.5GHz or faster
RAM: 4GB or more
Hard disk space: 500MB available or more**

* The requirements are for normal use and do not include resource intensive features like Burst Mode
** Additional hard disk space may be required to store generated data by the application.

Prerequisites

Internet access is not required for automatic installation of .Net Framework.
.Net Framework 4.8 or higher is required.

Installation Procedure

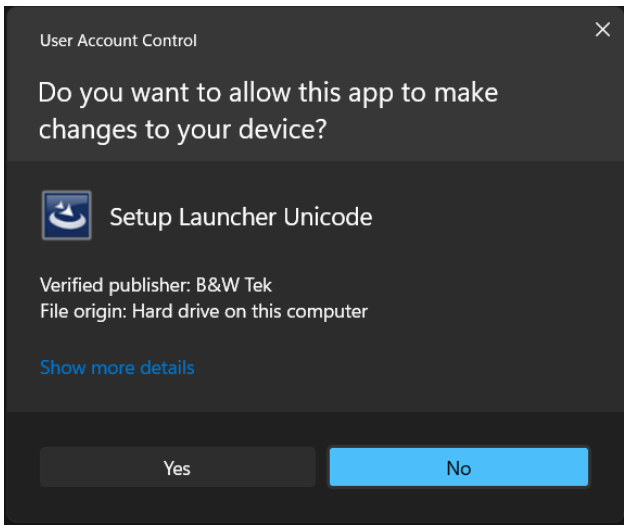
- **For computers with BWSpec already installed, it is highly recommended to uninstall the existing one and execute the following steps.**
- Locate BWSpec software installation package and copy the entire package to local computer. **Installation through network is not recommended and success is not guaranteed.**
- Locate proper setup.exe from either 32bit or 64bit subfolder, double left click to begin the installation process. User must have administrator rights for installation.
- After software installation, **DO NOT** open the BWSpec program.
- Connect the spectrometer to the PC via a USB Cable.

- Install the Hardware Driver(s) for the spectrometer.
- After hardware driver installation, open/run the BWSpec program.

3 RUN BWSPEC

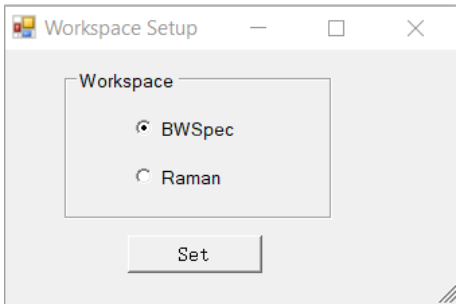
Double click the BWSpec icon on the desktop: 

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



Click **Yes** to continue.

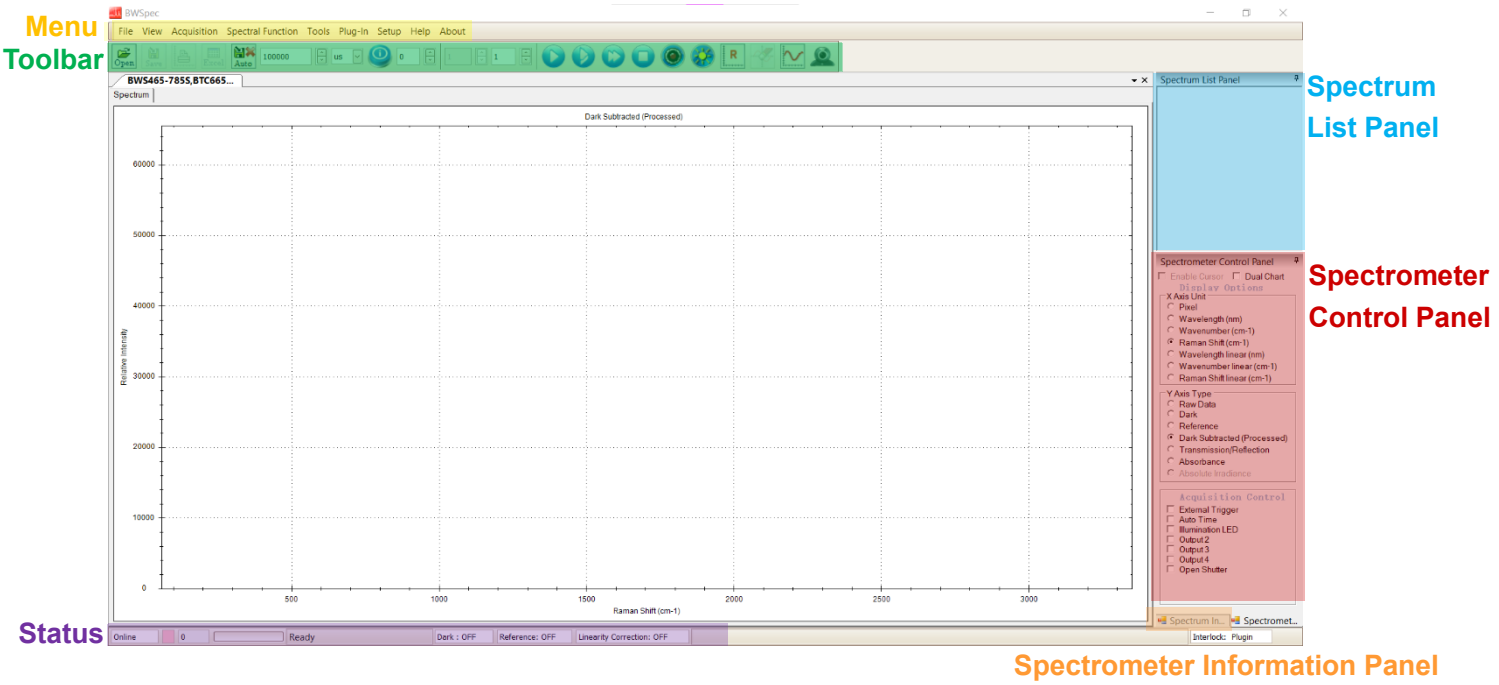
The **Workspace Setup** window will open, prompting the user to choose a workspace based on their unit and application.



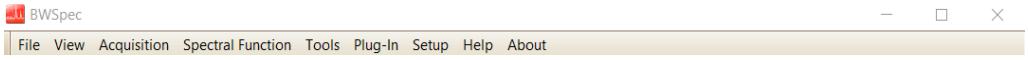
If you are unsure, choose the default **BWSpec** workspace and click **Set**. This option may be changed later within the main program; Setup → Workspace.

4 MAIN WINDOW

Presented below is a brief visual overview of the BWSpec 4 main window. The main toolbars, panels and tabs are highlighted; refer to the corresponding section for more detailed information.

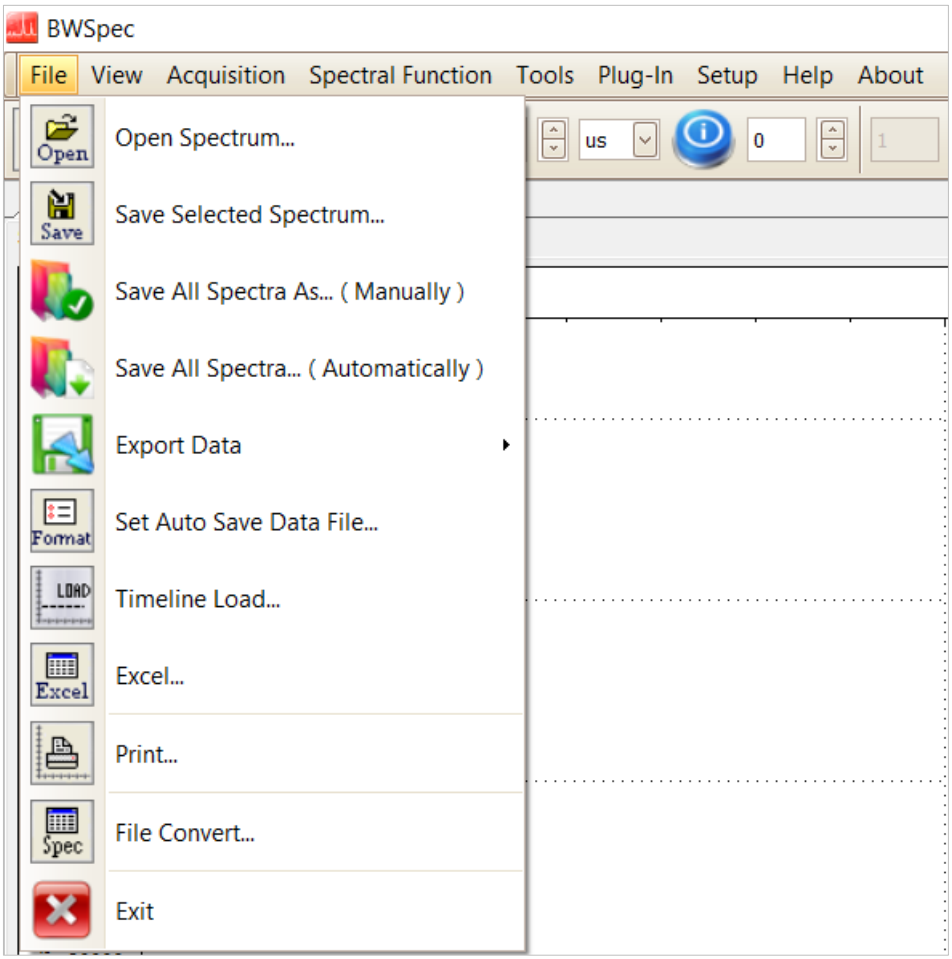


5 MENU BAR



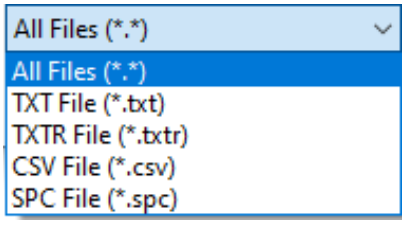
The following sections are detailed descriptions of the dropdown menus available for each menu option in the BWSpec 4 Menu Bar.

6 FILE



Open Spectrum…  Open Spectrum...

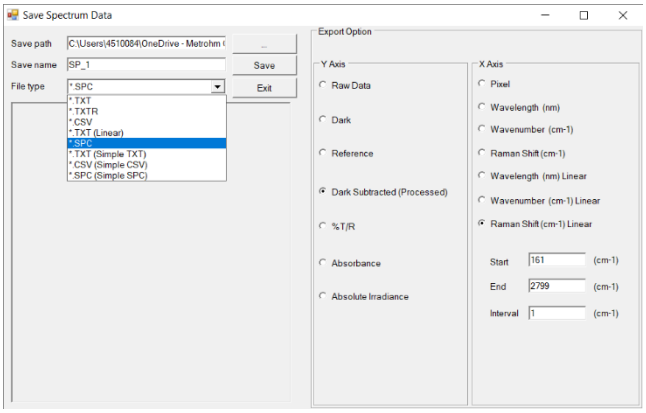
Load a previously saved spectral file into the main graph.
Available in the following formats:



TXT File (*.txt) including BWSpec TXT and simple TXT
TXTR File (*.txtr)
CSV File (*.csv) including BWTek raw CSV, LIMS CSV and simple CSV
SPC File (*.spc) with XY two series data which could be saved through BWSpec or from other instruments and software

Save Selected Spectrum…  Save Selected Spectrum...

Save the spectrum selected in the **Spectrum List Panel**.
Used to save data of selected spectrum from BWSpec in the following formats:
***.TXTR** – this is set as default - .TXTR files contain information about the spectrometer, acquisition parameters, data processing, applied Ratio 1, 2, and 3, and data from all axis types. This file type includes the most information and can be saved as all other data formats.
***.TXT** - .TXT files contain information about the spectrometer, acquisition parameters, and data from all axis types.
***.CSV** - .CSV files contain information about the spectrometer, acquisition parameters, data processing, and data from all axis types. Compatible with Microsoft Excel.
***.TXT(Linear)** – same as .txt. However, the user may choose 'Save only the selected X and Y axis data' which will not contain any additional information.
***.SPC** – data is encrypted. SPC files are compatible with other Raman software
***.Simple TXT** – contains only one set of x-axis data in Raman Shift (cm-1) and one set of y-axis Dark Subtracted (Processed) data.
***.Simple CSV** – same as Simple TXT
***.Simple SPC** – same as Simple TXT

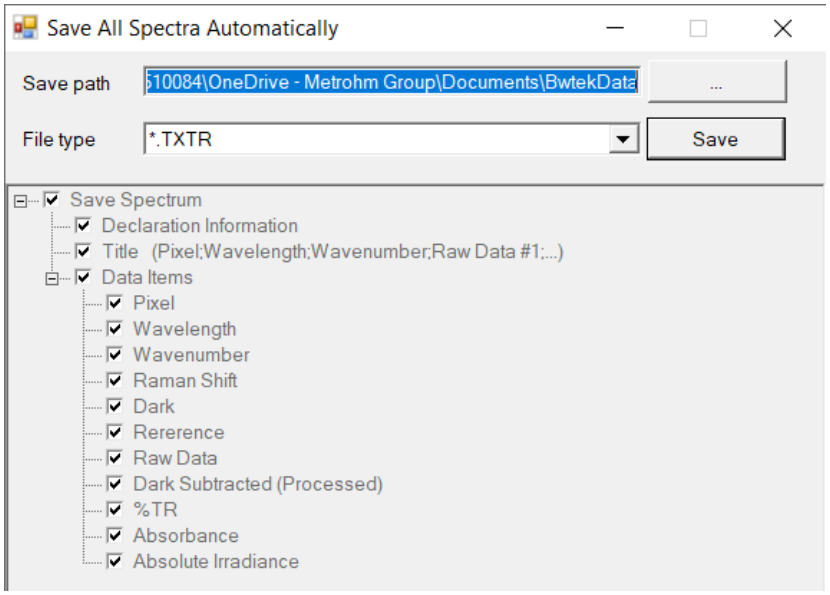


Save All Spectra As… (Manually)

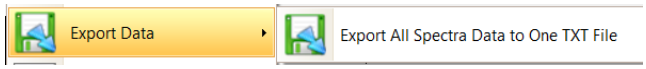
Saves all spectra in the **Spectrum List Panel** individually. User can change save name and file type for each spectrum. A new Save Spectrum Data window will open for each spectrum.

Save All Spectra… (Automatically)

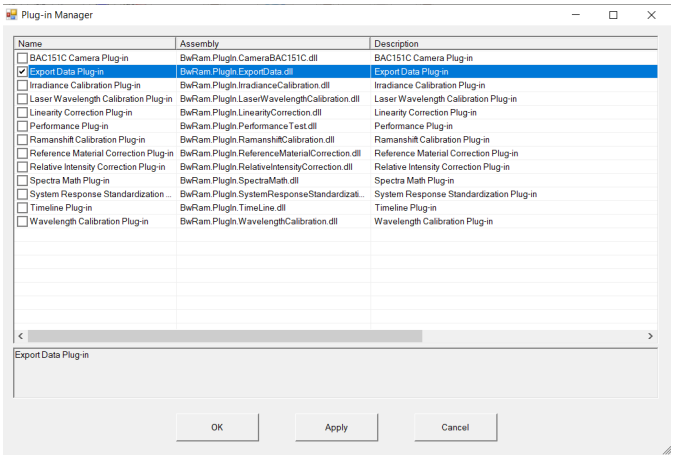
Saves all spectra in the **Spectrum List Panel** at the same time. The data will be saved with the name shown in the Spectrum List Panel. All files will be saved as the same, user-selected file type. The active spectrum must be .txtr, .csv, or .txt formats or a measured spectrum for this feature to be enabled.



Export Data

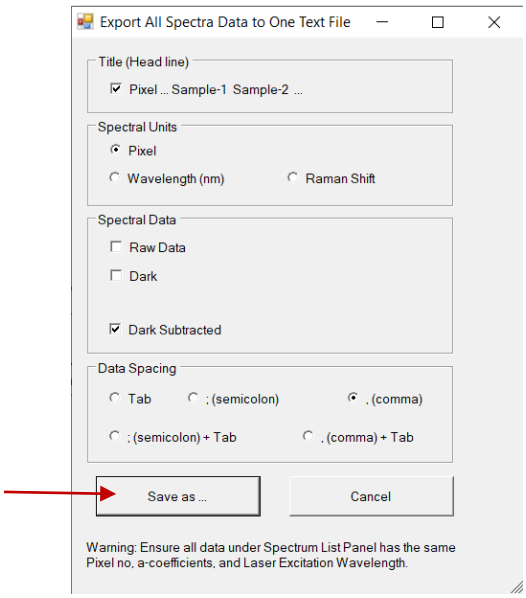


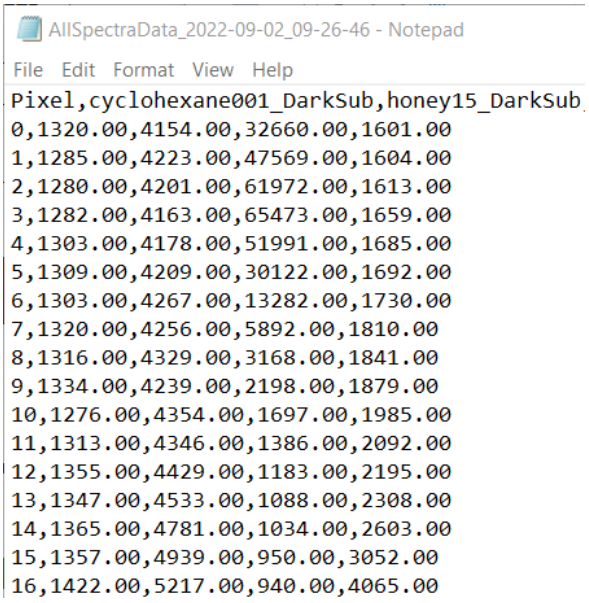
This requires plug-in turned on in Plug-In > Plug-In Manager:



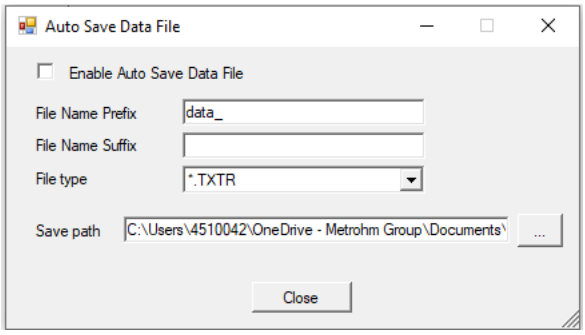
Export Data Plug-in

The **Export Data Plug-in** gives the function to export all spectral data into one text file.
Location: in the Menu Bar → File, choose **Export Data→ Export All Spectra Data to One TXT File**.
Select the data information to be exported, and click **Save As**.
All selected Spectra will be exported and saved to a text file. The active spectrum must be .txtr, .csv, or .txt formats or a measured spectrum for this feature to be enabled.





Set Auto Save Data File…  Set Auto Save Data File...



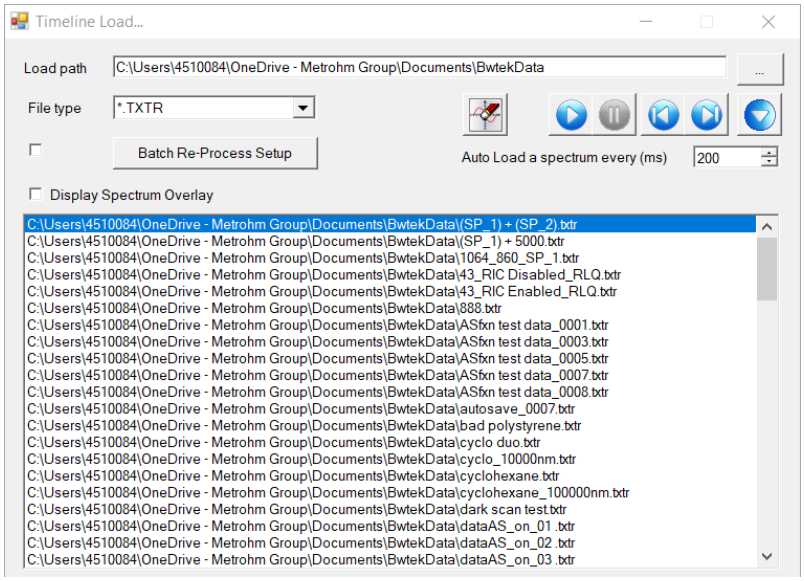
This is the setting to automatically save all scanned data to a designated folder.

When this is enabled, all functions under Tools are disabled.

When this is enabled, dark scan is mandatorily required for this first scan and when integration time is changed.

When this is enabled, Reference button is disabled.

Timeline Load…  Timeline Load...



This function allows user to re-run previously saved Timeline series with the ability to re-define data processing and analysis. May be used with Batch Re-Process to reprocess the data as it loads into BWSpec.

Excel

Excel...

Export the active/selected single spectrum from the **Spectrum List Panel** to an Excel sheet.
The active spectrum must be a Measured spectrum or BWSpec TXT or TXTR format if it is an opened spectrum.
Only one active spectrum can be exported to Excel at one time.
Data is opened in Excel when the export is successful.
Compatible with all Excel versions.

Print…

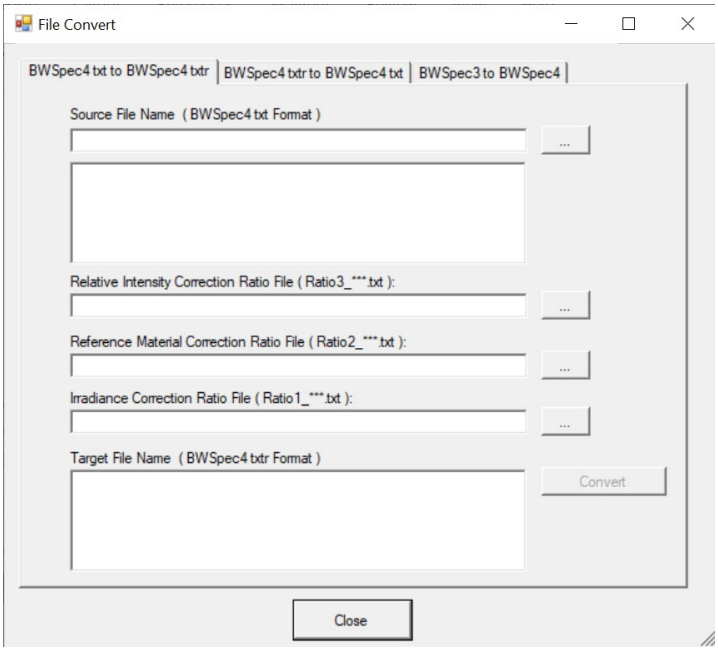

Print...

Show **Print Preview** window with the displayed data and header information for the active spectrum.
Add watermark, Save As, Print and etc.

File Convert…

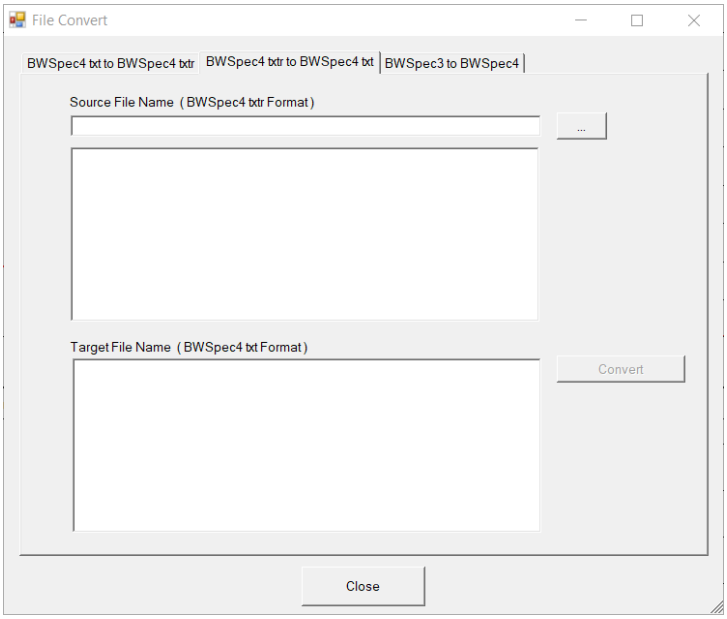
File Convert...

Convert all spectral files of the same format under a selected folder into another format.
Convert BWSpec4 *.txt files to BWSpec4 *.txtr file type.
All three Ratio files for the same instrument the data was collected on must be loaded for the conversion to have the corrections applied.
Any processing done in the *.txt file is not recorded in Data **Pretreat** section.

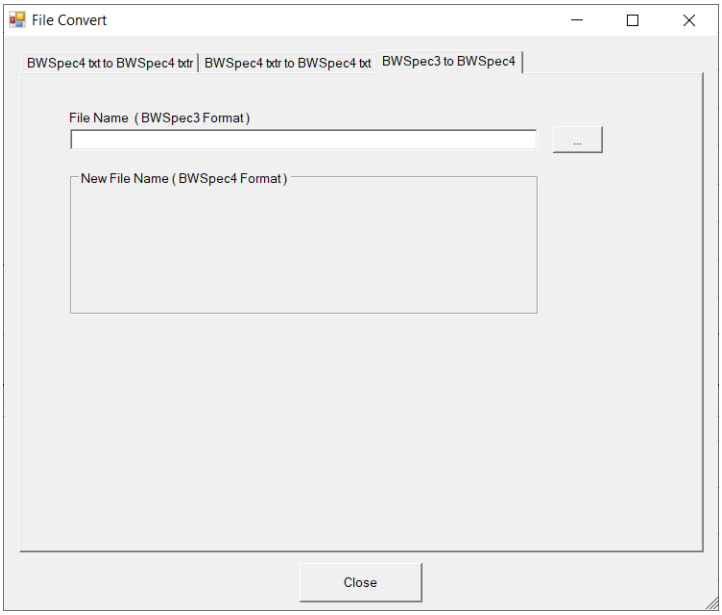


Convert BWSpec4 *.txtr files to BWSpec 4 *.txt file type.

Convert BWSpec3 data files which may contain multiple spectra (up to 3) into individual BWSpec4 compatible files.



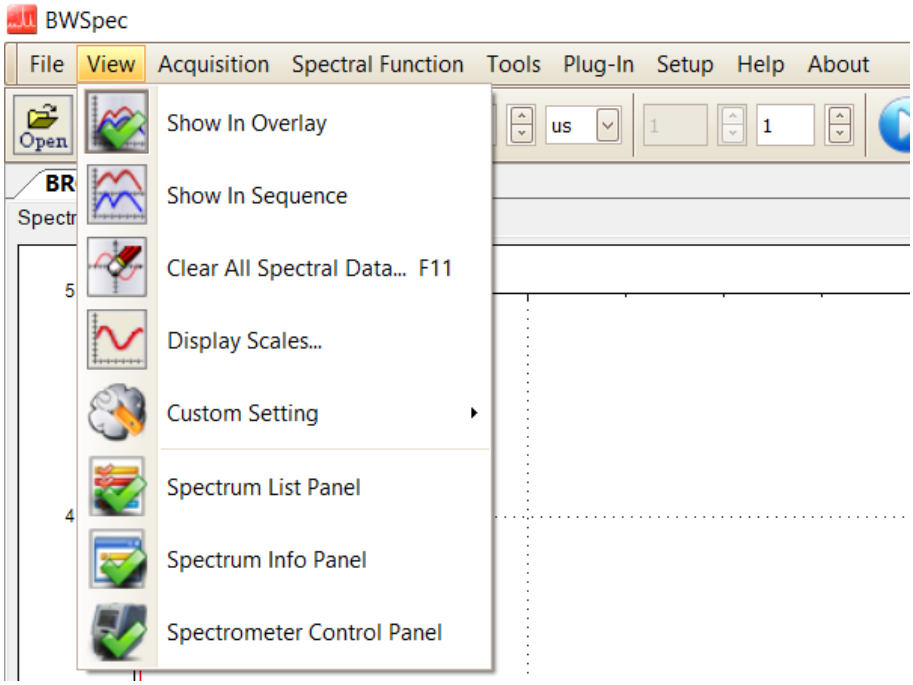
Convert BWSpec3 file format to BWSpec4



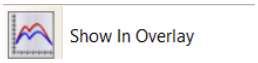
Exit

Closes the BWSpec program.
You will be prompted to save any unsaved or modified spectra.

7 VIEW

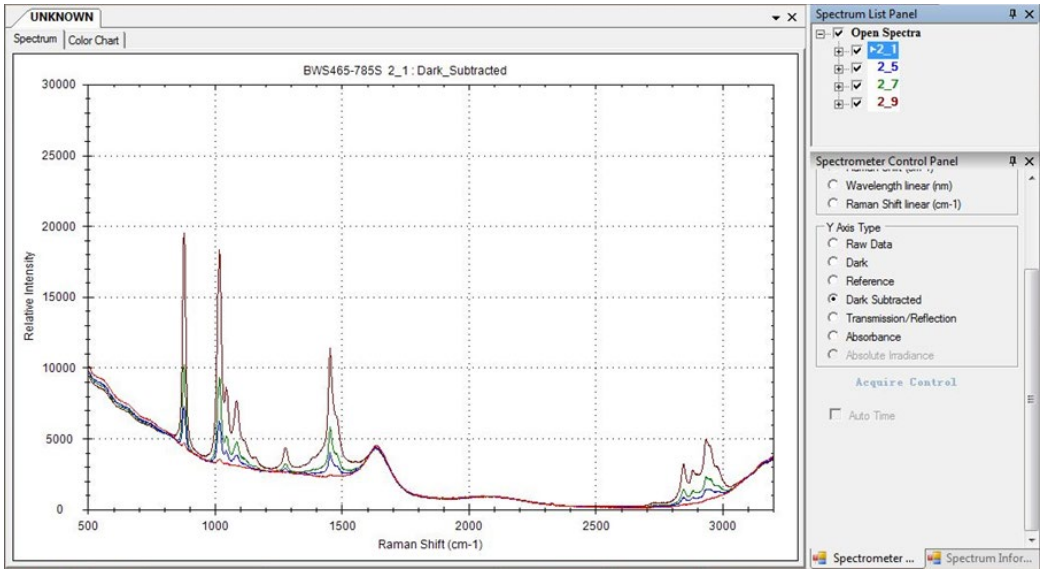


Show In Overlay



When viewing more than one spectrum, an overlay of each spectrum in the **Spectrum List Panel** will be displayed in the main graph.

When enabled (default) a green checkmark is shown.

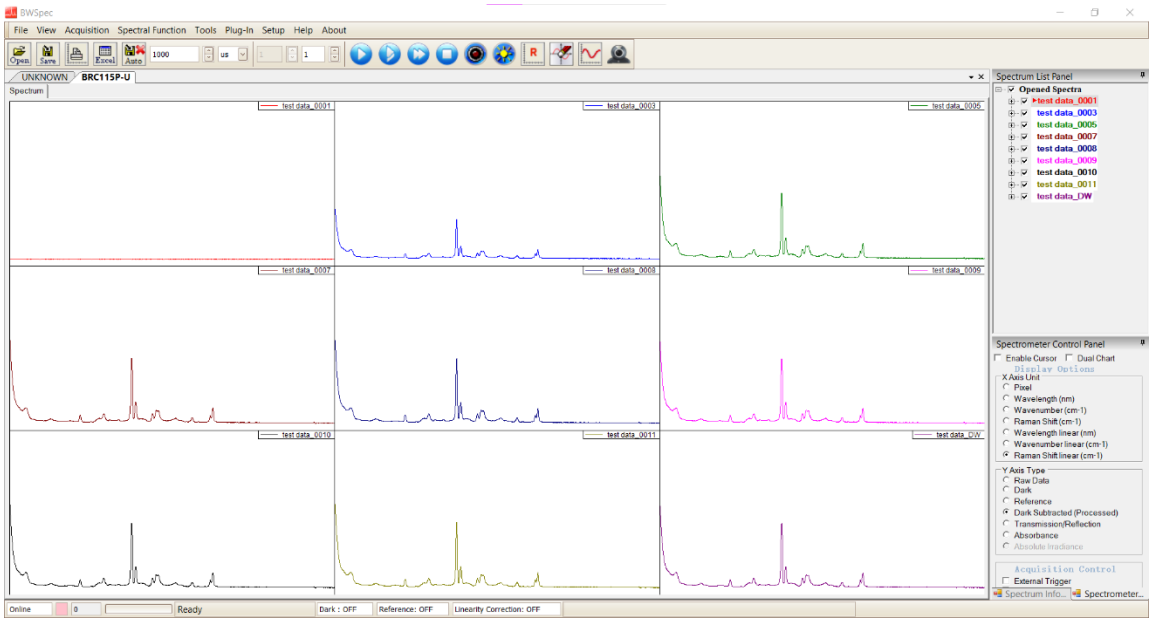


Show In Sequence

When viewing multiple spectra, individual graphs will appear in the order they are listed in the **Spectrum List Panel**.

When enabled, a green checkmark is shown. 

Show in Overlay and **Show in Sequence** are mutually exclusive options.

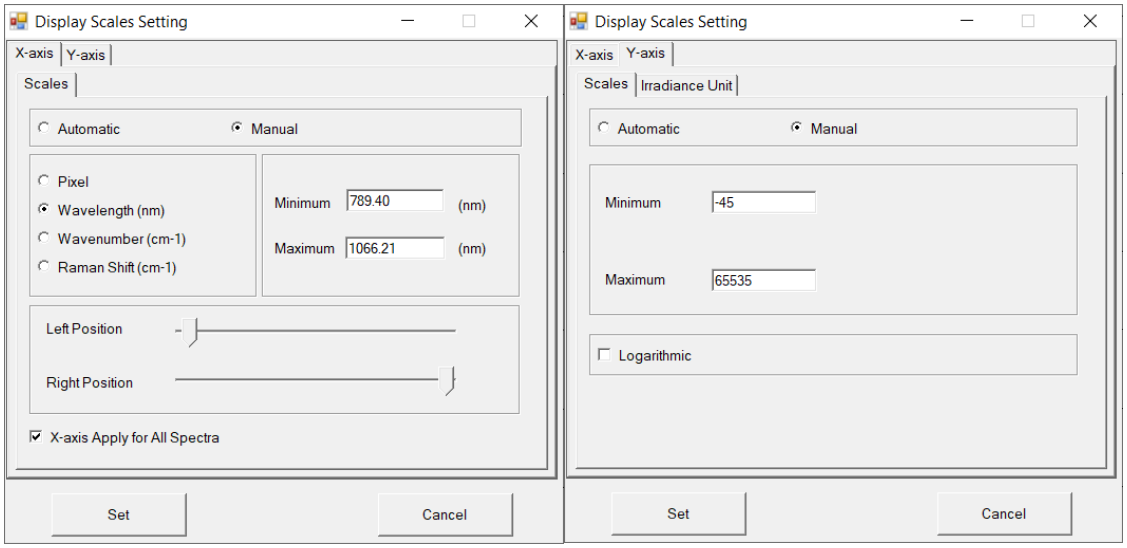


Clear All Spectral Data…

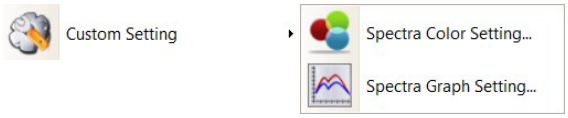
Remove all spectra from the **Spectrum List Panel** and display area.

Display Scales…

The **Display Scales Setting** window shows the graphing window's X-axis and Y-axis settings.
X-axis scale settings are based on the default calibration settings for the spectrometer.
Using **Automatic** Scales will auto-adjust the graph and axis to fit the current displayed data.
While using **Manual** Scales, the **X-axis** may be changed by typing in a **Minimum** and **Maximum** into the boxes, or by moving the slider for the **Left Position** and **Right Position**.
Check the **X-axis Apply for All Spectra** to apply changed settings to all spectra in the **Spectrum List Panel**.
Click the **Set** button to apply the selections to the graph. In the **X-axis**, the selection will be applied to the nearest pixel.



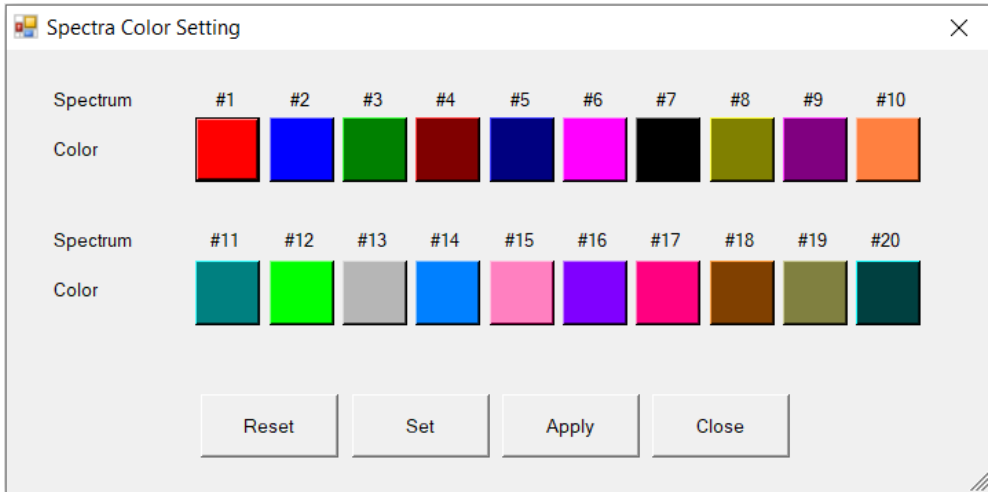
Custom Setting



Display settings for the main graph window.

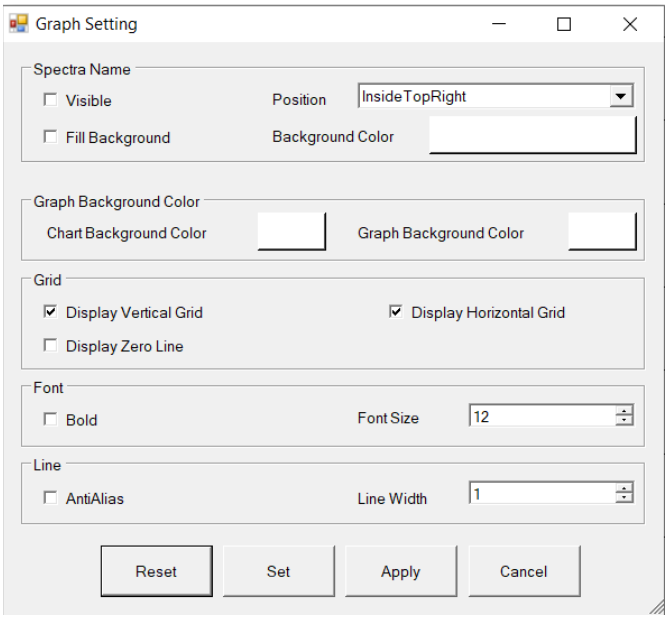
Spectra Color Setting…

Opens a **Spectra Color Settings** window where the spectrum color order for overlays can be set / adjusted. The sequence is based on spectra 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 and adjusted to create a customized graph.



Spectrum List Panel


Spectrum List Panel

There are two types of spectra: Measured spectra and Opened spectra. Measured spectra are data files just collected from online instrument. Opened spectra are loaded offline data.

Toggles On/Off display of the **Spectrum List Panel** on the right side of the display.

Spectrum with the flag symbol before the name is the "**active**" spectrum. 

The most recent active measured spectrum will be overwritten if a new single scan is taken (Acquire One Spectrum)

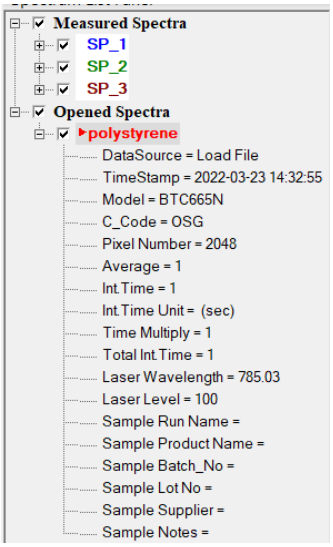
A new measured spectrum will be added to the list if an Overlay scan is taken (Acquire Overlay)

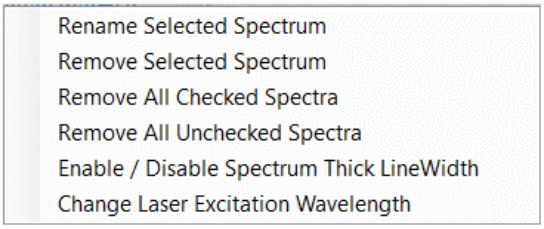
Dark and Reference scans will be updated to active Measured spectrum.

Expanding the **+** will give information on the spectrometer and settings used to collect the spectrum.

When enabled (default) a green checkmark is shown. 
Spectrum List Panel

Refer to Spectrum Information Panel for more details.





Right-click menu:

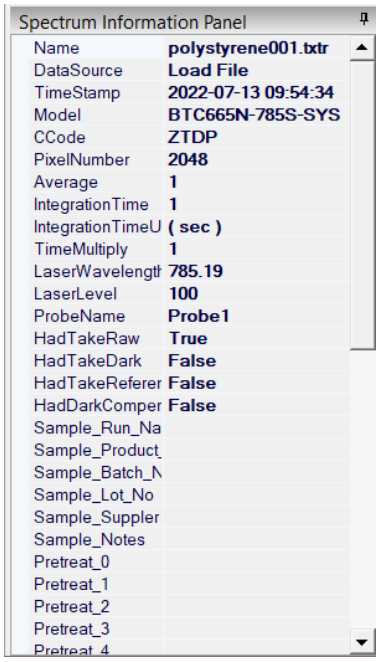
Select a spectrum name and then right click. Menu appears with the options:

Rename Selected Spectrum (rename the selected spectrum without saving it), Remove Selected Spectrum (deletes the selected spectrum from the Spectrum List Panel) , Remove All Checked Spectra (deleted all spectra from the Spectrum List Panel that have a checkmark next to them), Remove All Unchecked Spectra (deletes all spectra from the Spectrum List Panel without a checkmark next to them), Enable / Disable Spectrum Thick LineWidth (changes the line thickness of the spectrum trace), Change Laser Excitation Wavelength (user can manually adjust the laser wavelength from what it was set to at the time of acquisition).

Spectrum Information Panel

 Spectrum Info Panel  Spectrum Info Panel

Toggles On/Off display of the **Spectrum Information Panel**.
Displays spectrum details including spectrometer and laser information.
Any processing steps used are listed in the **Pretreat_#** section
When enabled (default) a green checkmark is shown.

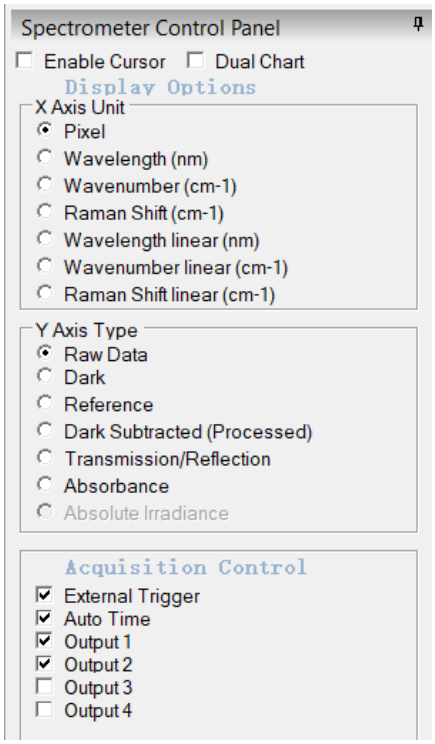


Spectrometer Control Panel

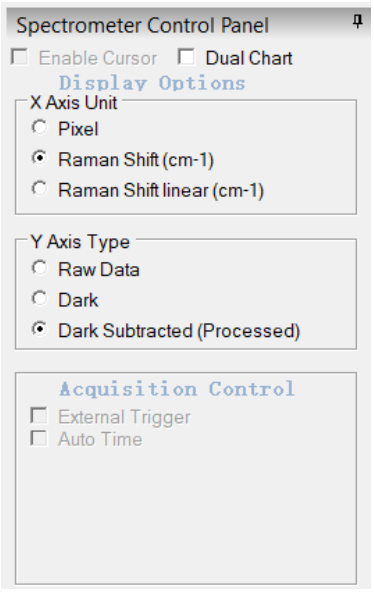
 Spectrometer Control Panel  Spectrometer Control Panel

Toggles On/Off viewing of the **Spectrometer Control Panel**.
The availability of the listed options depends on the **Workspace** selected.
When enabled (default) a green checkmark is shown.

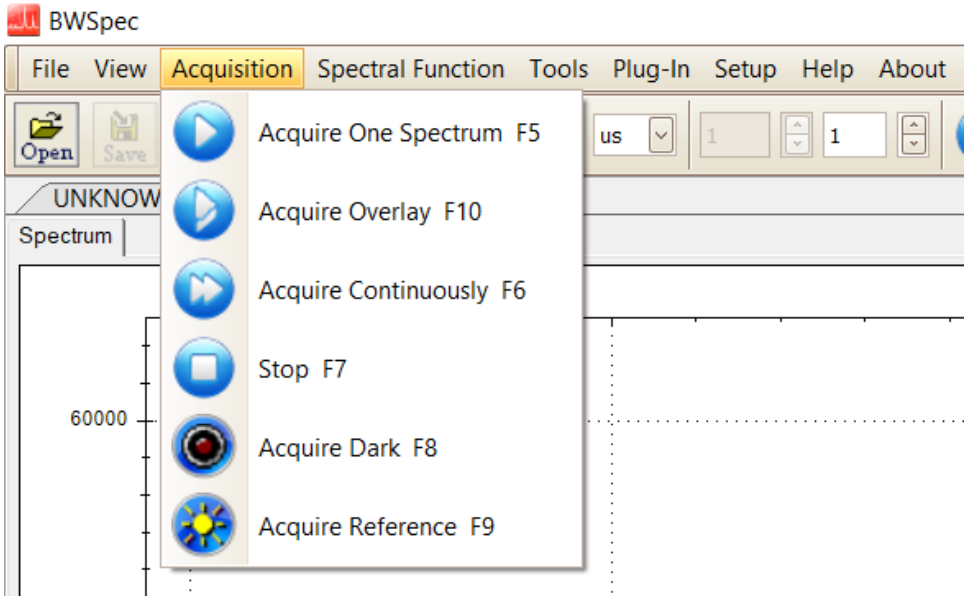
BWSpec Workspace



Raman Workspace



8 ACQUISITION



Acquire One Spectrum

Acquires a single spectrum from the spectrometer and displays it on the graph.
The data is viewable on the **Raw Data Y Axis Type.**

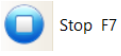
Acquire Overlay

Acquires a single spectrum and displays it over top of the previously displayed spectra.
Note that the previously taken spectra can no longer be edited.
The data is viewable on the **Raw Data Y Axis Type.**

Acquire Continuously

Data is continuously displayed in the graph from the spectrometer with no delay between scans. The data is viewable on the **Raw Data Y Axis Type.**

Stop



Stops acquisition while using **Acquire Continuously**.

Acquire Dark

Acquires a single spectrum which is stored as the **Dark** array.
The Dark array is viewable in the **Dark Y Axis Type**.

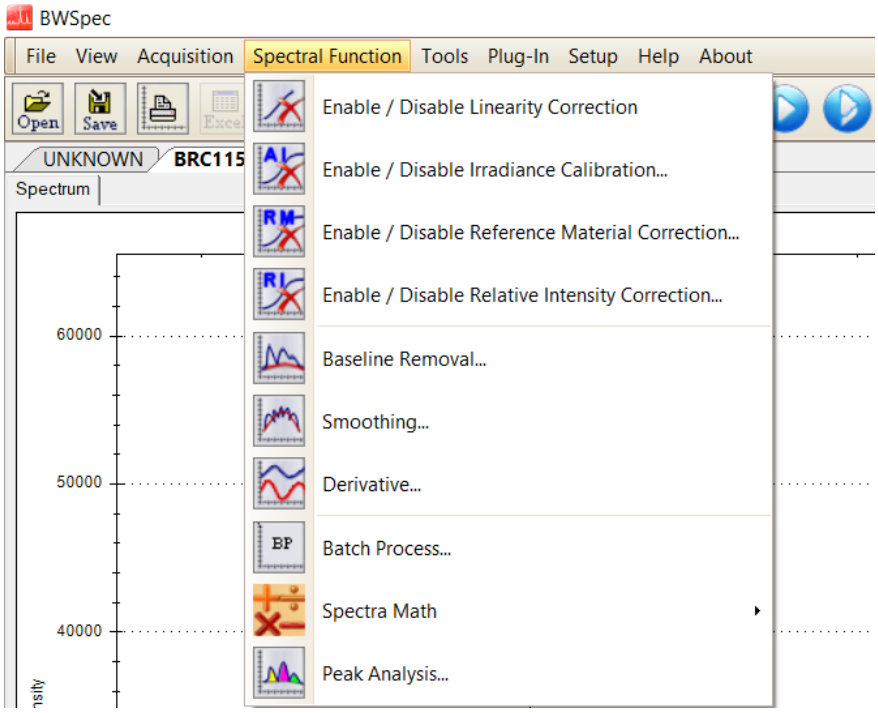
Acquire Reference

Acquires a single spectrum which is stored as the **Reference** array.
The Reference array is viewable in the **Reference Y Axis Type**.

Acquisition Tips

A **Dark Spectrum** is used to subtract the contribution (dark noise) of the sensor itself or noise from environment. This is carried over until a new dark spectrum is acquired. **Every time when integration time and/or average are changed, dark spectrum must be collected again.**
A measured spectrum is unfinished when it is just acquired. It becomes Finished after it is saved or after a new spectrum is measured.
To ensure data integrity, BWSpec prevents the measurement of a new spectrum when the last measured spectrum is unfinished, for example, when in **Raman Workspace**, the integration time of the signal and the dark spectrum are not the same. If you are unsure if the raw and dark integration times same, attempt an **Acquire Overlay**. If they have different integration times, BWSpec will alert the user that the integration time of the raw and dark do not match.
Use the **Auto Dark** feature in Hardware Setup → Common to take a Dark scan after each Acquisition.
If the last **Measured Spectrum** is unfinished and is selected, it can be overwritten by a new measurement. No other spectrum can be overwritten by a new measurement except a new spectrum.

9 SPECTRAL FUNCTION



Items under Menu -> Spectral Function are:

- Enable / Disable Linearity Correction
- Enable / Disable Irradiance Calibration…
- Enable / Disable Reference Material Correction…
- Enable / Disable Relative Intensity Correction…
- Baseline Removal…
- Smoothing…
- Derivative…
- Batch Process…
- Spectra Math
- Peak Analysis…

  Since the **Raw Data**, **Dark**, and **Reference** data are protected, functions that alter the data are disabled if the active **Y Axis Type** is set to one of these types. Such functions include Baseline Removal, Smoothing, Derivative, Batch Process and Spectra Math. **Peak Analysis** does not alter the data and is enabled on these **Y Axis Types**.

Please note that the ability to use certain functions may be superseded if Experiment is enabled. Check the loaded Experiment configuration file for details if it is enabled.

Linearity Correction

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

A typical detector array may 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.

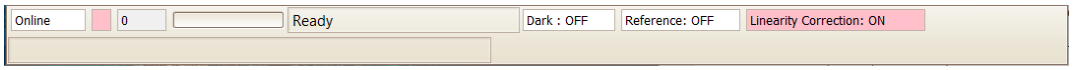
Linearity Correction must be conducted by the factory in order for the Linearity Correction Coefficients to be saved into device EEPROM. Refer to section under Menu->Tools for details if interested. "Linearity Correction" is a service option to be ordered when purchasing the spectrometer or through a service request.

Linearity correction can be configured in Menu->Spectral Function->Enable/Disable Linearity Correction…or in Experiment Setup.

In the menu, Linearity correction is off by default and can be enabled when instrument is online:

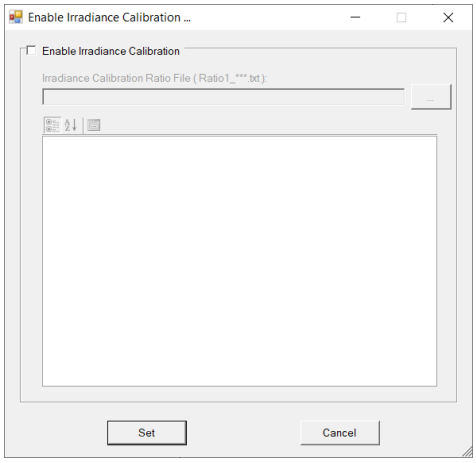
Linearity coefficients are read from spectrometer EEPROM.

When it is enabled, status on the bottom will show Linearity Correction is ON.



Irradiance Calibration

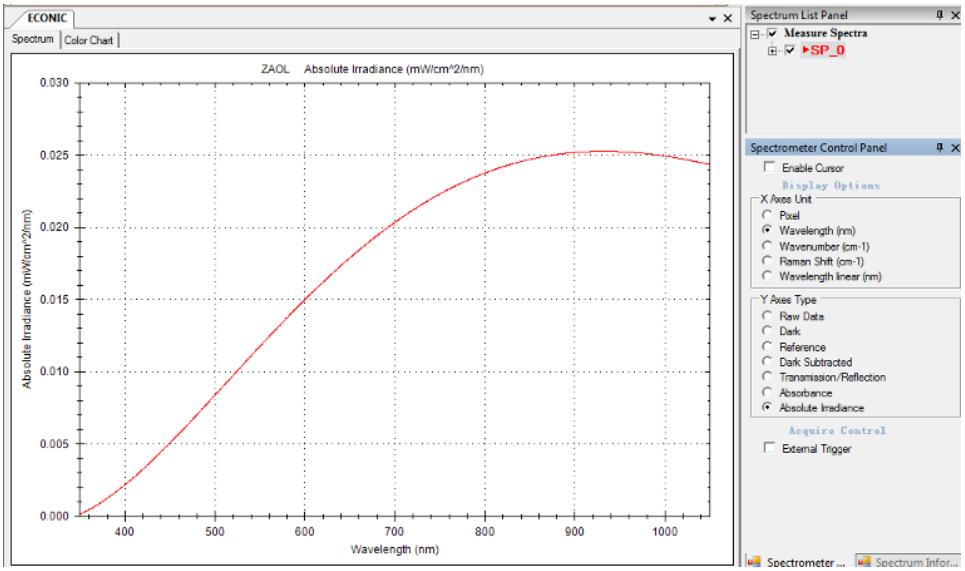
This calibration is to convert the spectrum response from relative intensity to absolute photometric response for measurement of photometry and colorimetry for a light source.



Irradiance Calibration can be configured in Menu->Spectral Function->Enable/Disable Irradiance Calibration…or in Experiment Setup. To enable this calibration, user has to load file ratio1_xxx.txt where xxx is cCode of spectrometer.

When Irradiance Calibration is enabled, after a scan has been taken, 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.



Reference Material Correction

 Enable / Disable 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.

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

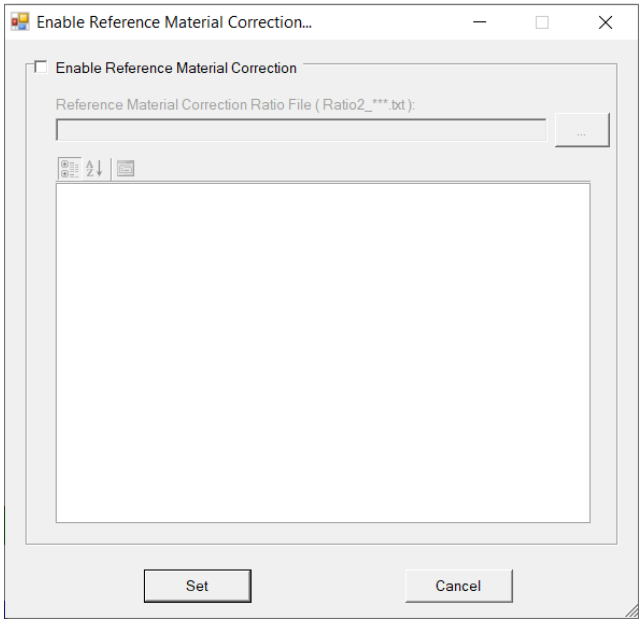
If we define %Rs (non-correction) as the sample percent reflectance at a given wavelength:

%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.

Reference Material Correction can be configured in Menu->Spectral Function->Enable/Disable Reference Material Correction …or in Experiment Setup. To enable this correction, user has to load file ratio2_xxx.txt where xxx is cCode of spectrometer.

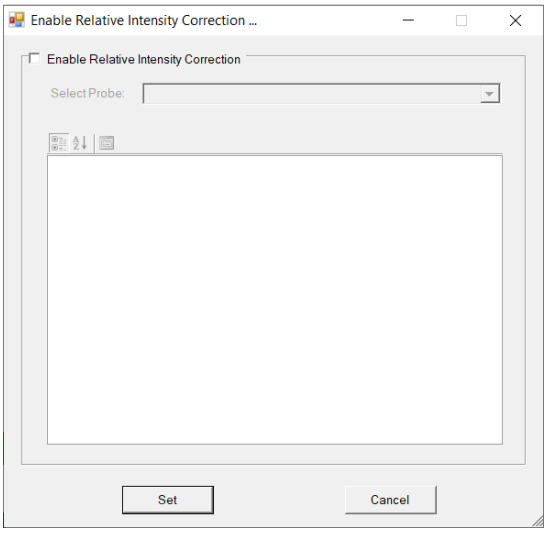


Relative Intensity Correction

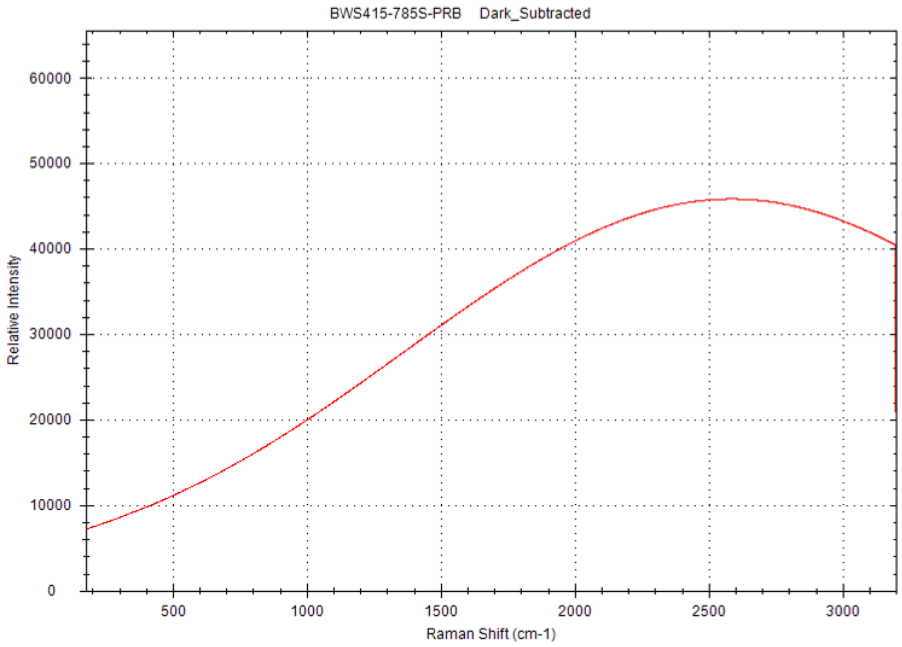
Relative Intensity Correction is specific for Raman spectrometer users. Its purpose is to correct unique relative spectral responses against a traceable standard for individual spectrometers. The corrected spectral response of a Raman spectrometer makes meaningful comparisons between data obtained from different instruments possible.

The 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(the latest is SRM2242a) when a 532nm excitation laser source is used and SRM2244 when a 1064nm excitation laser source is used. Refer to website for more details: SRM Definitions | NIST

Relative Intensity Correction can be configured in Menu->Spectral Function->Enable/Disable Relative Intensity Correction …or in Experiment Setup. To enable this correction, user must choose probe to load file ratio3_xxx.txt where xxx is cCode of spectrometer.



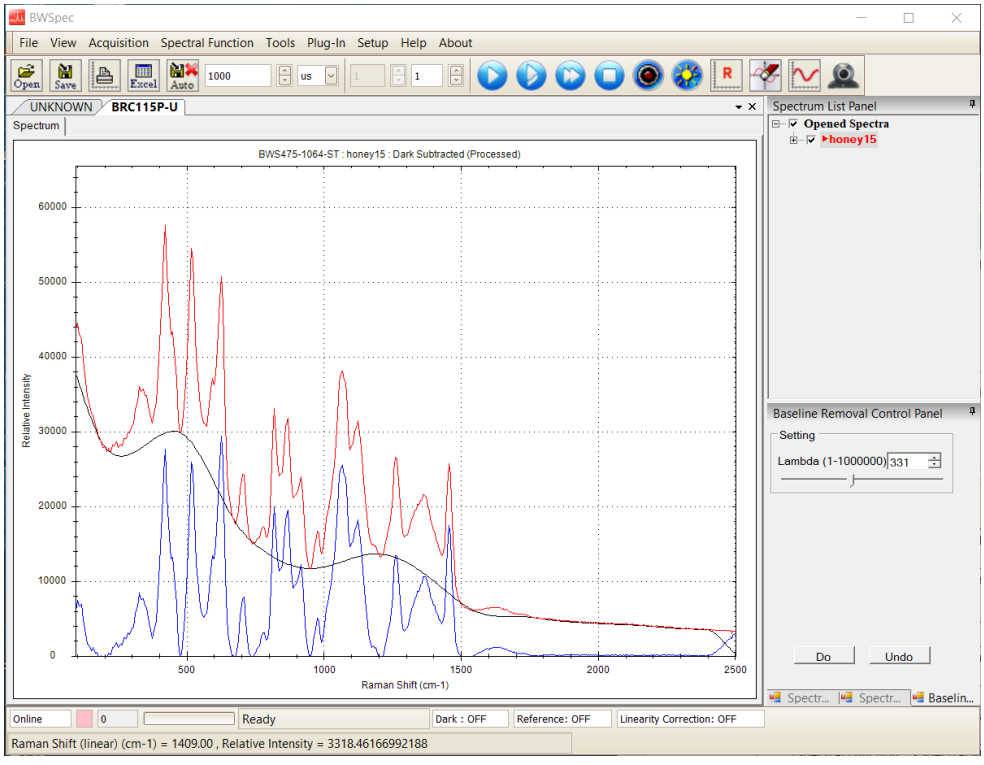
To change the Relative Intensity Correction setting of saved spectra, use the Batch Re-Process function.



Baseline Removal

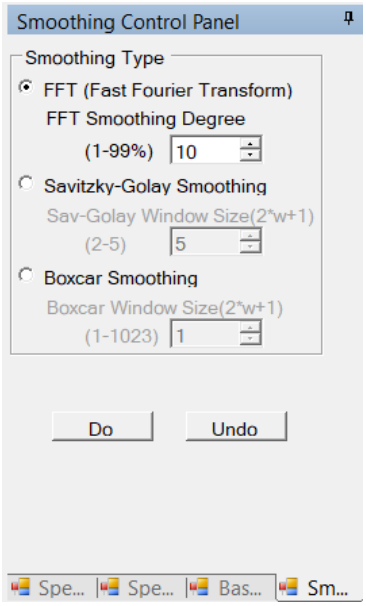
The **Baseline Removal** function is used to perform baseline correction. This helps remove spectrum background to correct for fluorescence, baseline curvature, noise, or ambient light.
This function is disabled when the **Y Axis Type** is set to **Raw Data**, **Dark**, or **Reference**.

A display window with three spectra will be displayed: raw spectrum (red), automatically fitted background curve (black), and the spectrum after background removal (blue). The color of the raw spectra reflects its color in the **Spectrum List Panel**.
The lambda factor can be adjusted by moving the slider bar at the top, or by typing in the **Lambda** box. This manipulates the auto fitted background to achieve the desired baseline removal result. Click **Do** to apply changes to the main graph.



Smoothing…  Smoothing...

Opens a **Smoothing** window for applying smoothing processing to all Checked spectra.
This function is disabled when the **Y Axis Type** is set to **Raw Data**, **Dark**, or **Reference**.
When clicked, a Smoothing Panel will appear on right panel:



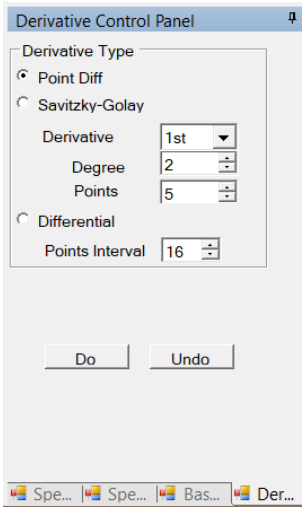
FFT (Fast Fourier Transform)
FFT Smoothing can be applied to the original spectrum using a smoothing factor of 1-99%.
The smoothing factor needs to be carefully selected so as not to cause a distorted spectrum.

Savitzky-Golay Smoothing
Savitzky-Golay Smoothing can be applied to the original spectrum with a window size setting from 2-5.
This is a commonly used smoothing method with less chance to cause distortion and degradation to the spectral resolution. A higher window size causes a greater degradation to 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 to preserve the needed spectral information.

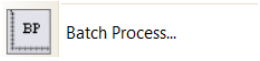
Derivative…  Derivative...

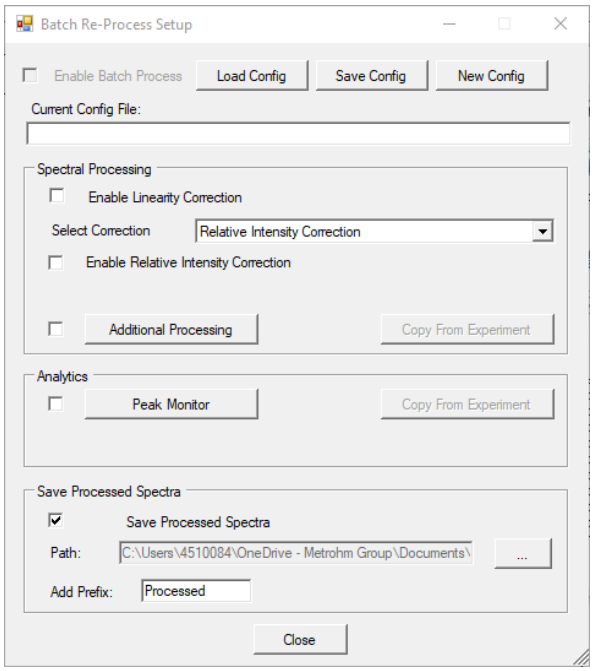
Opens the **Derivative Control Panel** for applying derivatives to all displayed spectra.
This function is disabled when the **Y Axis Type** is set to **Raw Data**, **Dark**, or **Reference**.
When clicked, the Derivative Panel will appear on right panel:



Point Diff: This computes the first derivative of the spectrum by the difference in the y response between two points on the x-axis.
Savitzky-Golay: the user can choose the derivative order, the degree (of the polynomial fit), and the number of points over which to compute the derivative.
Differential: the user can set the point interval to use from 5 to 20.

Batch Process





Batch Process works like **Experiment Setup** but used to process or re-process loaded spectra in the **Spectrum List Panel**. Check to ensure only loaded spectra of the same file format are loaded for the best experience.

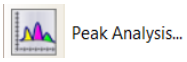
This function starts with the **Raw Data** (Raw and Dark in the file) of each spectrum. Each checked spectrum is processed according to the steps specified and the results are saved in the corresponding Processed Data block (called Dark Subtracted in the file). All other **Spectral Functions** start with the Processed Data block of each spectrum, performs the chosen function, and saves the results.

For example, if a Spectrum has previously been intensity corrected and smoothed, performing Spectral Function/Derivative on it will produce Processed Data that is intensity corrected, smoothed and then differentiated. Performing Batch Re-Process with “Enable Relative Intensity Correction” unchecked and a derivative step defined in Spectral Processing/Additional will produce a Processed Data that is differentiated on the Raw Data. These are reflected in the Pretreat sequence viewable in the **Spectrum Information Panel**.

Because different file types contain different data, it is impossible to apply one set of Re-Process steps to a set of Checked Spectra of mixed formats. So, if different file formats are selected, upon clicking “Batch Re-Process”, a warning message will display: “Selected Spectra are of different file formats. Please select spectra of the same format.”

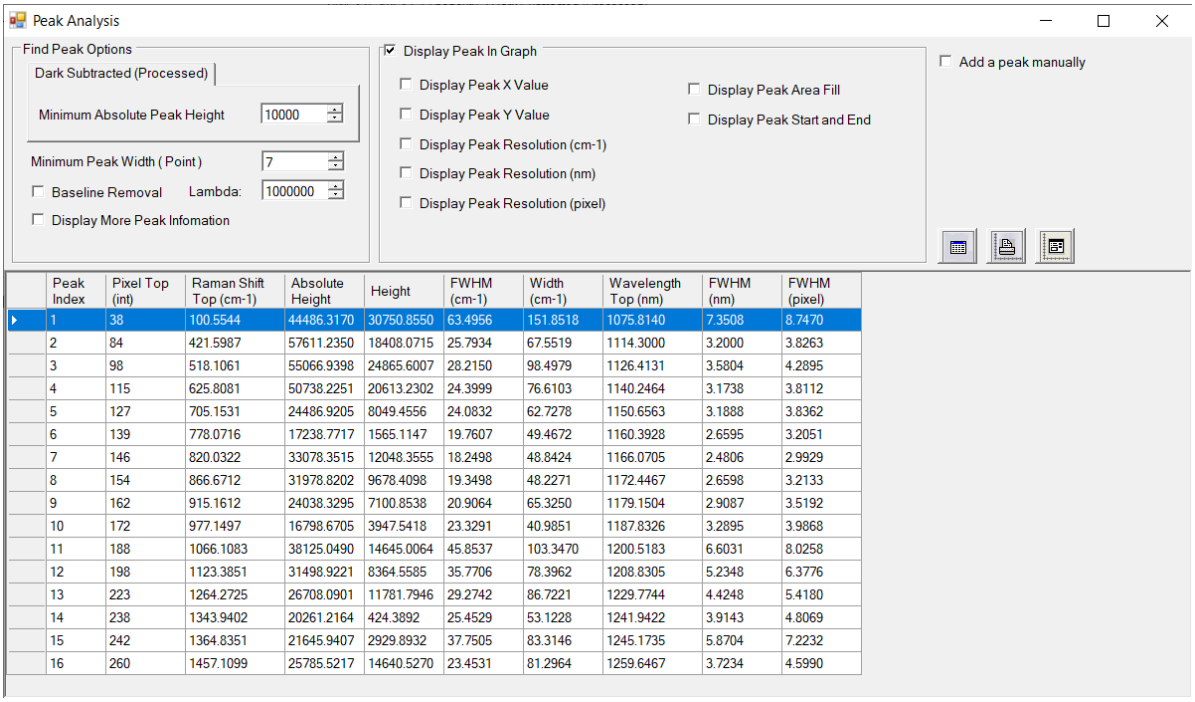
Spectral Processing includes both Instrumental Correction (found in Tools menu) and other spectral math functions. Some or all instrumental correction may be disabled due to file format.

If Checked Spectra are Measured spectra; when an Instrumental Correction requiring a ratio file is selected, the user must choose a Ratio file from disc.
If Checked Spectra are Opened Spectra of TXTR format, then all Instrumental Corrections are allowed, and if an Instrumental Correction requiring a ratio file is selected, the ratio data stored in each spectrum will be used to process the corresponding spectrum.
If Checked Spectra are Opened Spectra of TXT format, which does not have the ratio spectrum within, then all Instrumental Corrections are allowed, and if an Instrumental Correction requiring a ratio file is selected, the user must choose a Ratio file from disc.
If Checked Spectra are Opened Spectra of SPC (*.spc) format, which does not have the raw data, then all Instrumental Corrections are disabled. Processed data will overwrite existing data.
Analytics Settings may be imported from a currently loaded Experiment Setup configuration file using the **Copy From Experiment** button.
The Re-Processed data may be automatically saved if **Save Processed Spectra** is checked.
Click “Do” to execute the Batch Re-process, “Undo” to restore the original data. In case the **Save Processed Spectra** is checked, “undo” will also delete the files saved from the disc.
Any configuration created between the Batch Re-Process function in Timeline Load and this function may not be cross compatible. It is recommended to create a new configuration file for each mode if both modes are to be used
Refer to Experiment Setup section for details on processing features and a walk-through.

Peak Analysis… 

Information on peaks in the spectrum can be shown live in the software’s display window.
Automatic Peak Identification: Peak position is accurately determined by curve fitting, instead of using the position of the highest pixel.
In the top left-hand corner of the menu, input the value at **Minimum Absolute Peak Height** (threshold) and the **Minimum Peak Width**. All identified peaks are listed in the table.
This table provides detailed information on the identified peaks.
When **Baseline Removal** is checked, analysis results are based on the baseline subtracted spectrum. The Baseline corrected spectrum does not display or get applied.
Check the box for **Display Peak In Graph** and the identified peaks will be marked on the spectrum. Select the information to display in graph by checking the desired items.
Peaks may be added by checking **Add a peak manually**. Then go to the main graph and click and drag a box over the peak of interest.
Peak can be removed by right clicking this peak line then selecting **Delete This Peak**.
Select the **Report Export** button  to export table to an Excel sheet.
Select the **Print** button  o print a **Peak Analysis Report**, containing spectrometer information, the graph, and table.

Select the **Peak Field Setup** in **Print Report** button to change the field and to adjust the number of fields available in the Print Table.

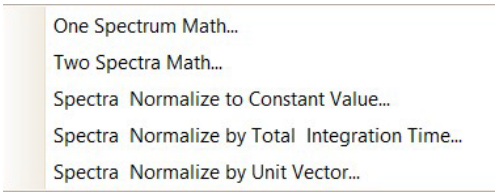


Peak Index	Pixel Top (int)	Raman Shift Top (cm-1)	Absolute Height	Height	FWHM (cm-1)	Width (cm-1)	Wavelength Top (nm)	FWHM (nm)	FWHM (pixel)
1	38	100.5544	44486.3170	30750.8550	63.4956	151.8518	1075.8140	7.3508	8.7470
2	84	421.5987	57611.2350	18408.0715	25.7934	67.5519	1114.3000	3.2000	3.8263
3	98	518.1061	55066.9398	24865.6007	28.2150	98.4979	1126.4131	3.5804	4.2895
4	115	625.8081	50738.2251	20613.2302	24.3999	76.6103	1140.2464	3.1738	3.8112
5	127	705.1531	24486.9205	8049.4556	24.0832	62.7278	1150.6563	3.1888	3.8362
6	139	778.0716	17238.7717	1565.1147	19.7607	49.4672	1160.3928	2.6595	3.2051
7	146	820.0322	33078.3515	12048.3555	18.2498	48.8424	1166.0705	2.4806	2.9929
8	154	866.6712	31978.8202	9678.4098	19.3498	48.2271	1172.4467	2.6598	3.2133
9	162	915.1612	24038.3295	7100.8538	20.9064	65.3250	1179.1504	2.9087	3.5192
10	172	977.1497	16798.6705	3947.5418	23.3291	40.9851	1187.8326	3.2895	3.9868
11	188	1066.1083	38125.0490	14645.0064	45.8537	103.3470	1200.5183	6.6031	8.0258
12	198	1123.3851	31498.9221	8364.5585	35.7706	78.3962	1208.8305	5.2348	6.3776
13	223	1264.2725	26708.0901	11781.7946	29.2742	86.7221	1229.7744	4.4248	5.4180
14	238	1343.9402	20261.2164	424.3892	25.4529	53.1228	1241.9422	3.9143	4.8069
15	242	1364.8351	21645.9407	2929.8932	37.7505	83.3146	1245.1735	5.8704	7.2232
16	260	1457.1099	25785.5217	14640.5270	23.4531	81.2964	1259.6467	3.7234	4.5990

Spectra Math

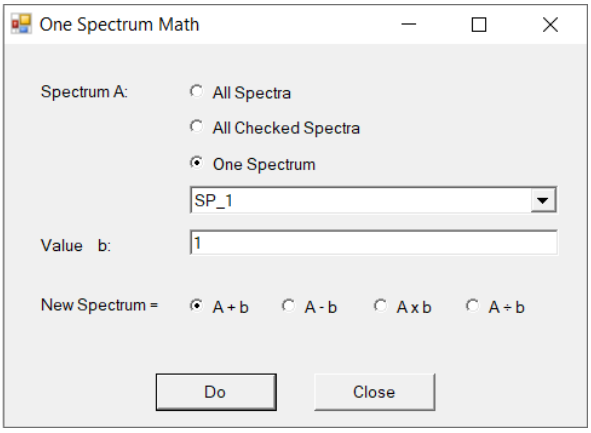
This function provides the ability to perform math functions on one, or multiple spectra.

Spectra math contains the following options:

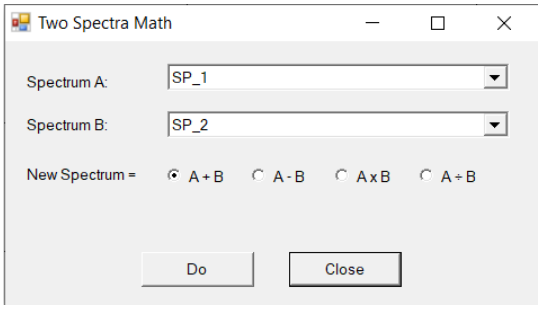


- One Spectrum Math
- Two Spectra Math
- Spectra Normalize to Constant Value
- Spectra Normalize by Total Integration Time
- Spectra Normalize by Unit Vector

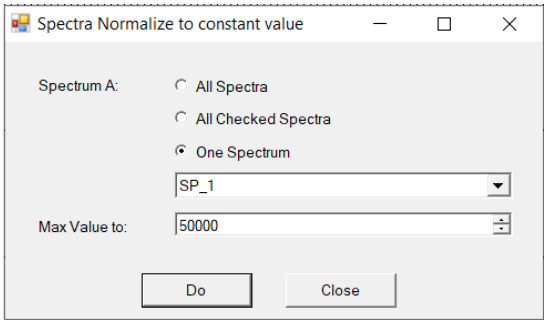
One Spectrum Math…



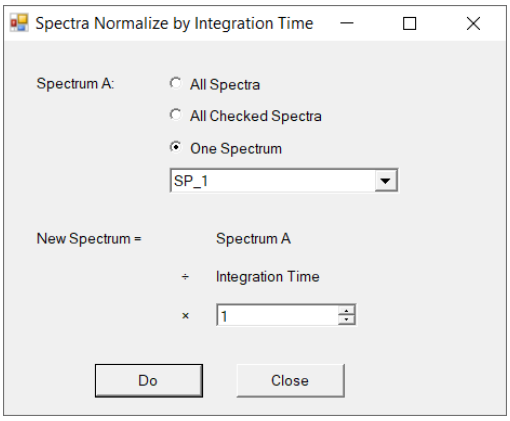
Two Spectra Math…



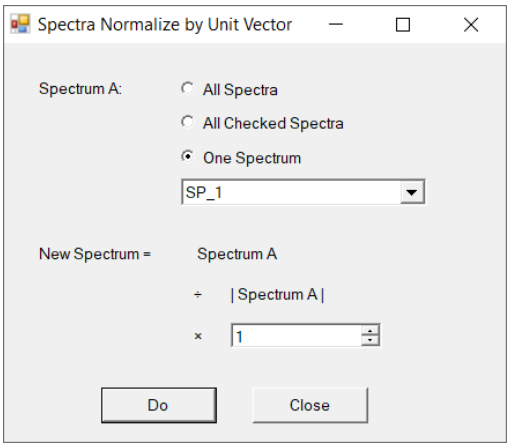
Spectra Normalize to Constant Value…



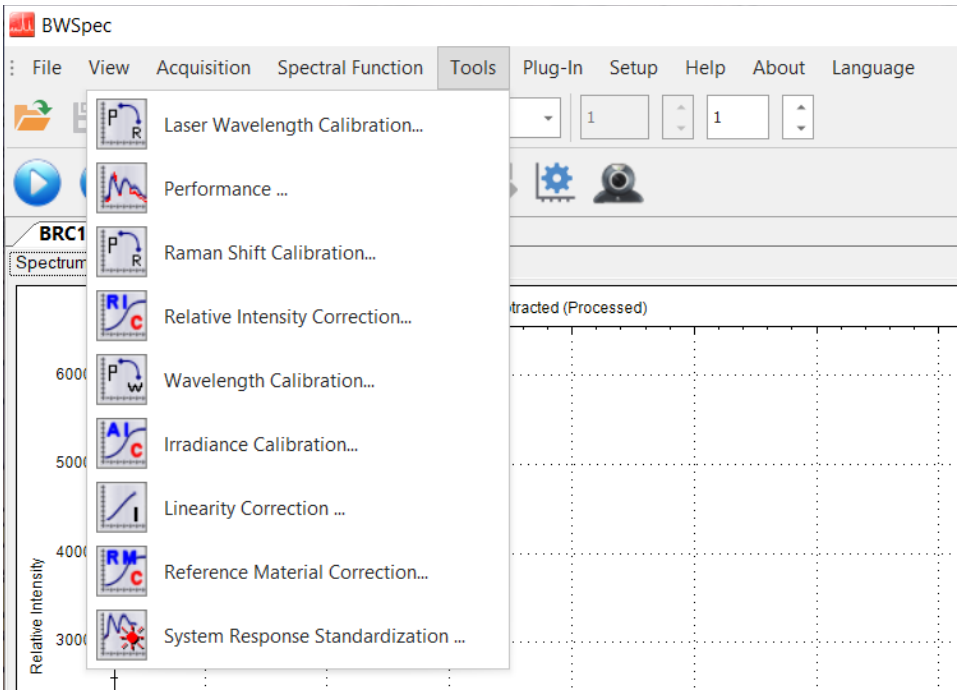
Spectra Normalize by Total Integration Time…



Spectra Normalize by Unit Vector

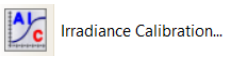


10 TOOLS



This menu provides a set of functions for instrument calibration and correction.

Irradiance Calibration
Laser Wavelength Calibration
Linearity Correction
Performance
Raman Shift Calibration
Reference Material Correction
Relative Intensity Correction
System Response Standardization
Wavelength Calibration

Irradiance Calibration 

This option is available only in the BWSpec Workspace. A NIST-Traceable Irradiance Standard light source is required. Follow instructions on screen to create irradiance calibration file ratio1.

Irradiance calibration can be configured in Menu->Spectral Function->Enable/Disable Irradiance Calibration… by loading proper ratio1 file or configured in Experiment Setup.

WARNING: This function is for advanced users only.

- 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.

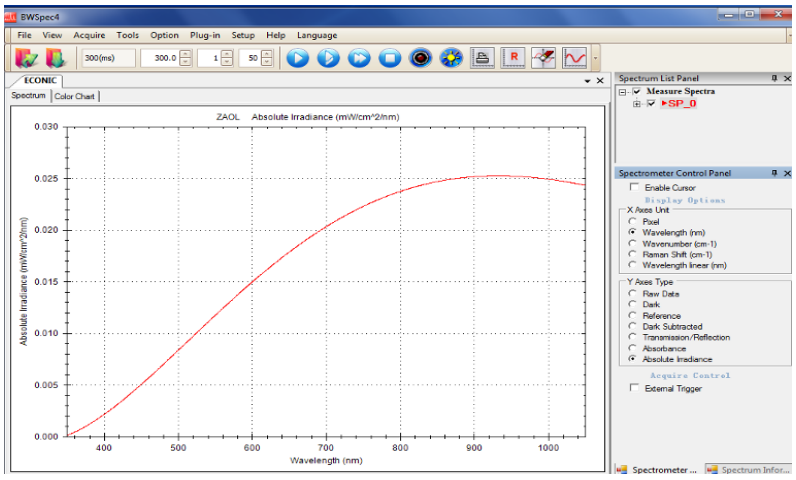
- It is also necessary to have the correct input optics for your spectrometer to collect the light, such as a fiber and an integrating sphere.

- 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).

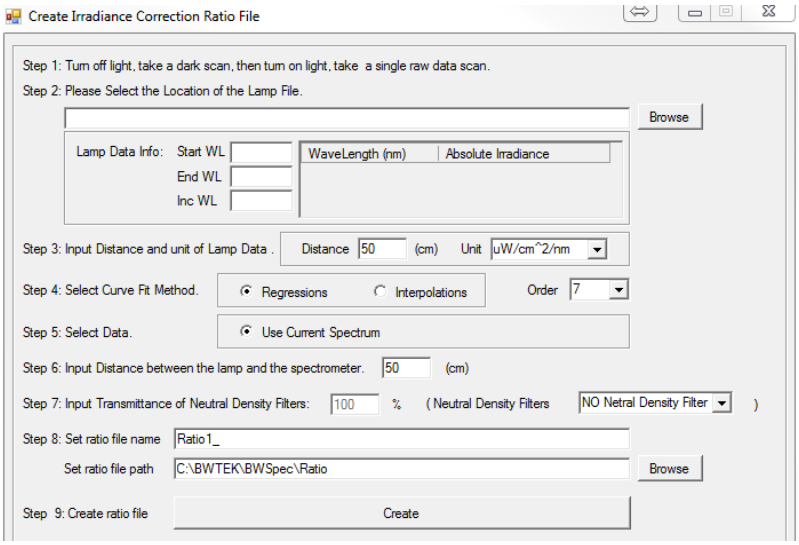
- Your setup conditions, distance from source, and lamp current must be as close as possible to what your NIST Certificate states to conduct a successful calibration. Ideally, the light source should not fill the spectrometer's entire angular aperture. The light source should illuminate the spectrometer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

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

Step 1: 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 2: Cover your light input aperture so that no light is gathered by your setup and take a ***Dark*** scan first. Then uncover the aperture and take a ***Raw*** scan. Select **Dark Subtracted (Processed)** Y-Axis Type to see the final data.



Step 3: go to Tools → Irradiance Calibration, click the Browse 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 way BWSpec can read it.



Step 4: Input the distance at which your Calibrated Light Source was originally calibrated. This information can be found 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 5: Choose either *Regression* or *Interpolation* to calculate Irradiance Ratio file.

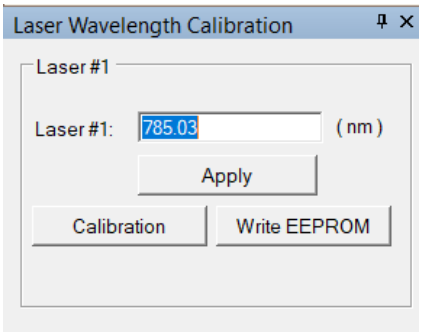
Step 6: Select **Use Current Spectrum** to use ***Dark Subtracted (Processed)*** data for calculation.

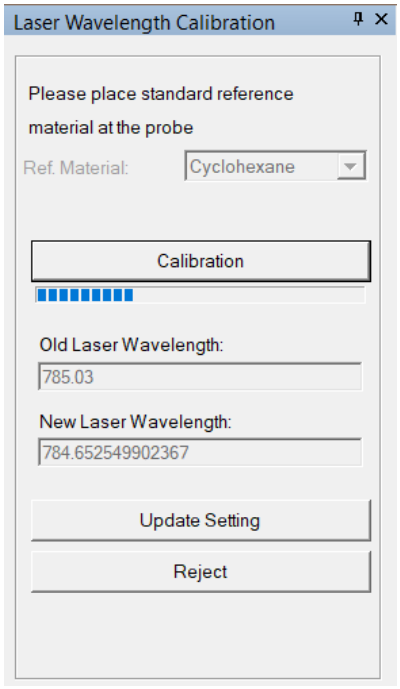
Step 7: Select the distance between your input optics and your certified light source in your current setup. Also, make sure to enter all calibration related information, such as additional optics used, into the dialog box.

Step 8: Input transmittance of neutral density filters.
Step 9: 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 10: Click **Create** to generate the **Irradiance Ratio File**.

Laser Wavelength Calibration

Laser Wavelength Calibration uses the peaks of cyclohexane to calculate the exact wavelength of the laser. Laser wavelength can be entered manually in the Laser Wavelength Calibration panel or in Hardware Setup > Laser Setup tab.
Press **Calibration** to open the Calibration screen. Place cyclohexane in front of the probe and press **Calibration** to begin. User can then **Update Setting** to the new wavelength value or **Reject** the change.





Linearity Correction

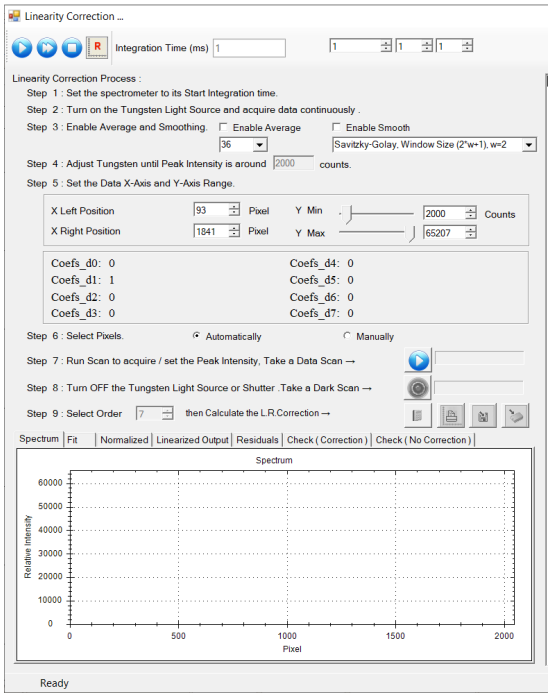
- Linearity correction will compensate for the detector array's nonlinear response by following a fitted response curve against received detector photons.
- A typical detector array may exhibit a nonlinear response with respect to incident photons at low light levels as well as when close to saturation. 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.
- Location: Menu Bar → Tools
- Linearity Correction must be conducted by the factory 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.

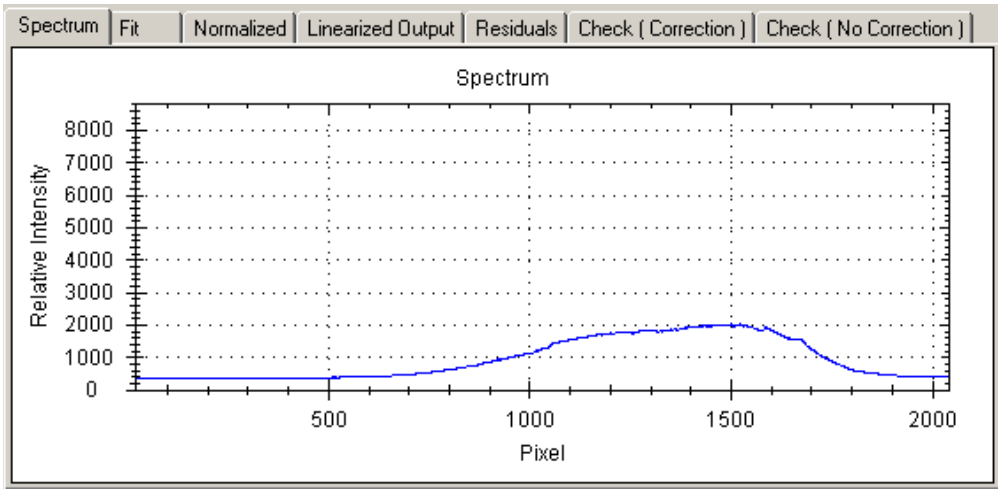
Activate Linearity Correction

- To activate linearity correction, go Setup > Experiment Setup and enable the checkbox. Linearity Correction only applies to **Dark Subtracted (Processed)** Y-Axis Type.

How to Conduct Linearity Correction

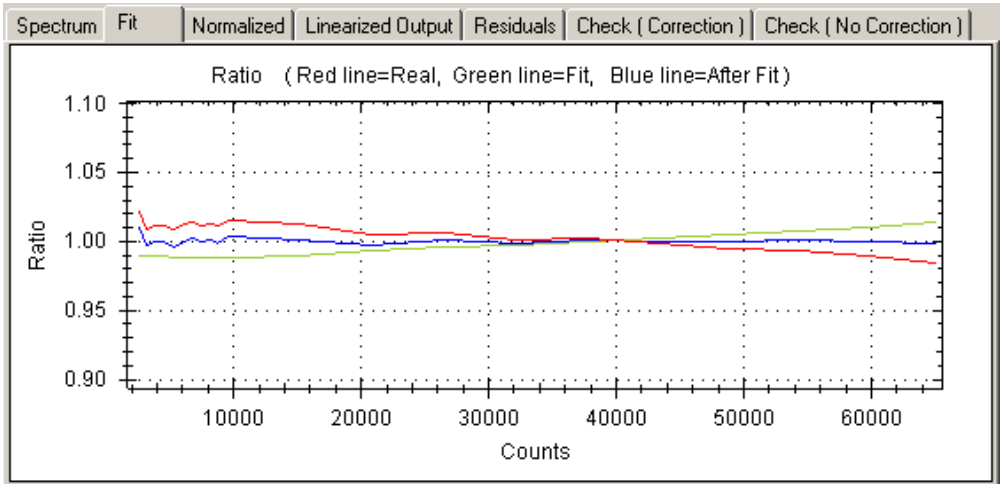
- For Advanced users, the linearity correction may be conducted at the customer site.
- From the Menu Bar, select Tools → Linearity Correction... The linearity correction window will appear. Follow Step 1 through Step 9 instructions in the window to proceed.





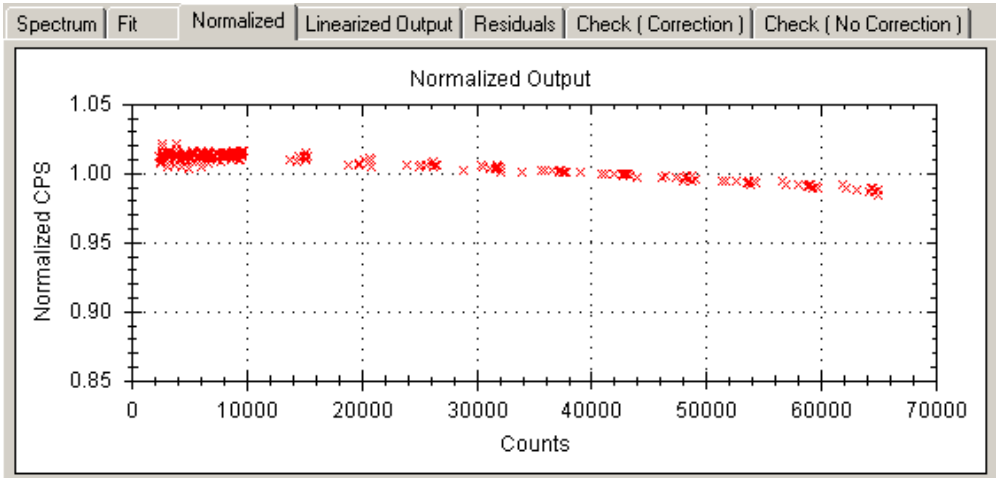
Spectrum

- 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.



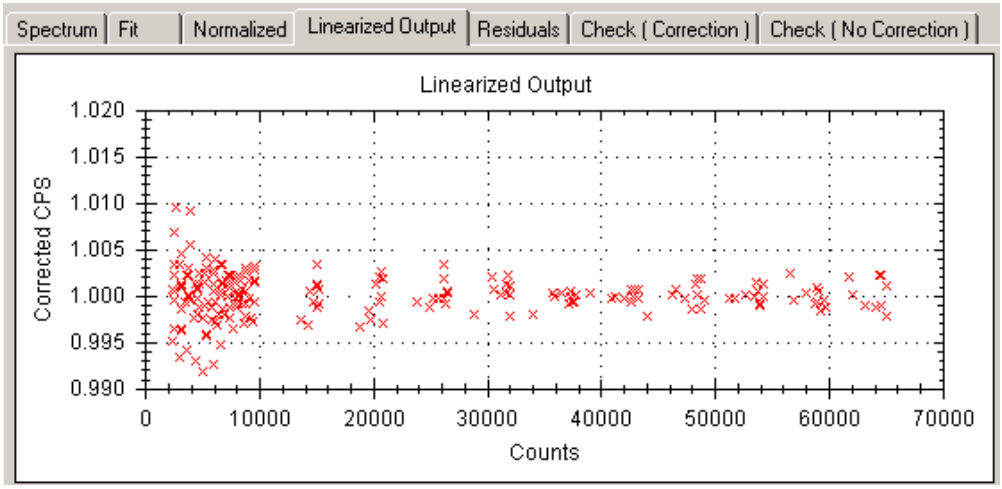
Fit

- Displays the fitting curve of the correction based on the Order (Step 9).
- Red is the Original, Green is the Fit curve, and Blue is the Corrected



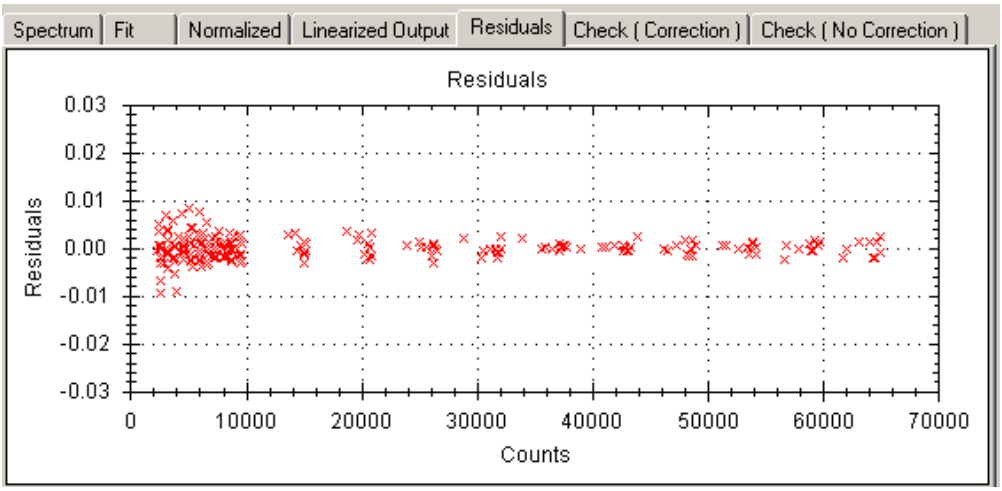
Normalized

- Displays the output before correction



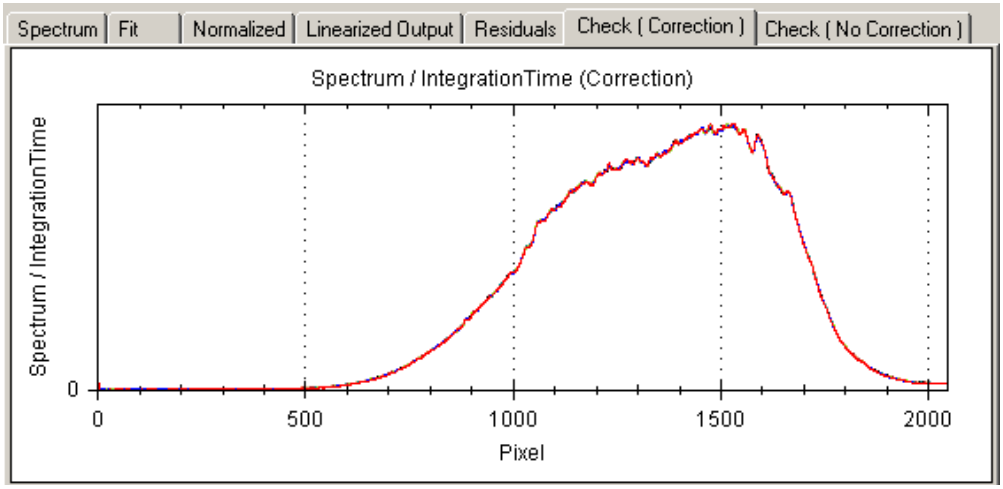
Linearized

- Displays the output after correction.



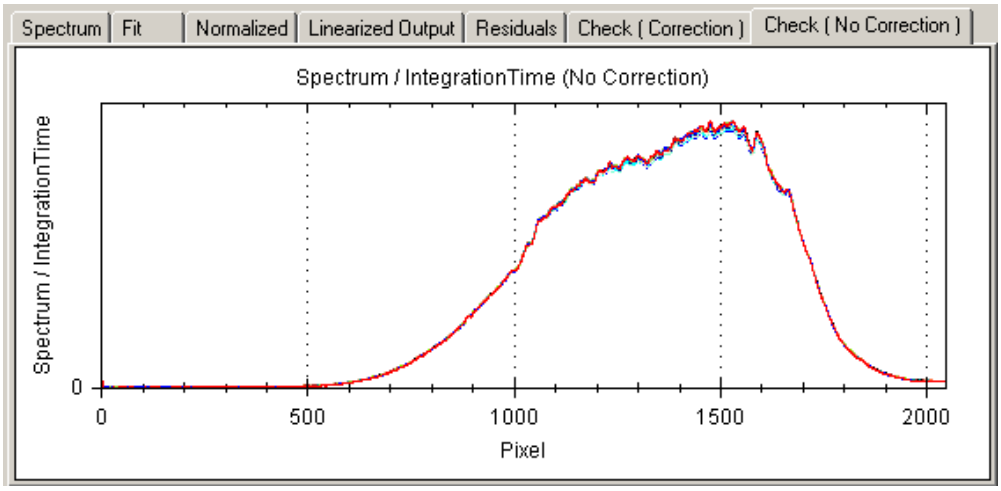
Residuals

- 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.

Performance…

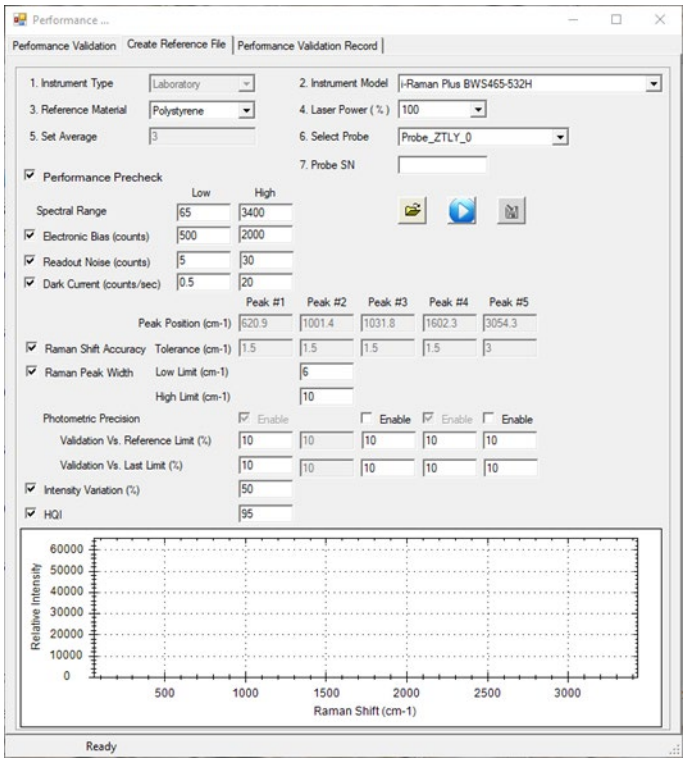
Performance is a function for all Raman instruments including laboratory Raman models. It is also applicable to DIY Raman setups but needs customized parameter settings.

Performance function is used to create a PVR (performance validation reference) file which is the reference for the performance validation test. Each instrument should have its own PVR file. We recommend user to recreate the PVR file after hardware or calibration changes such as the replacement of sampling accessories, spectrometer and laser modules, new Wavelength Calibration, Raman Shift Calibration or Laser Wavelength Calibration.

Performance validation implemented in BWTek software products is compliant with regulations from EP2.2.48, USP 858 and other related guidelines, and even more specifications are checked to have a higher control of system performance.

Even if the product is not used in a regulated environment, performing a regular performance validation is still strongly encouraged to guarantee the performance and also the reliability of output results.

Performance module is not available when status is offline.



Create Reference File

To create a PVR file, an instrument must be online. The connected model will be automatically identified and selected by the Instrument Model field. Instrument type will be Laboratory. Select the Reference Material used for the Reference file: Polystyrene, Acetaminophen, or Cyclohexane. Average and Laser Power can be set. Select the Probe to be used. Probe SN is not required.

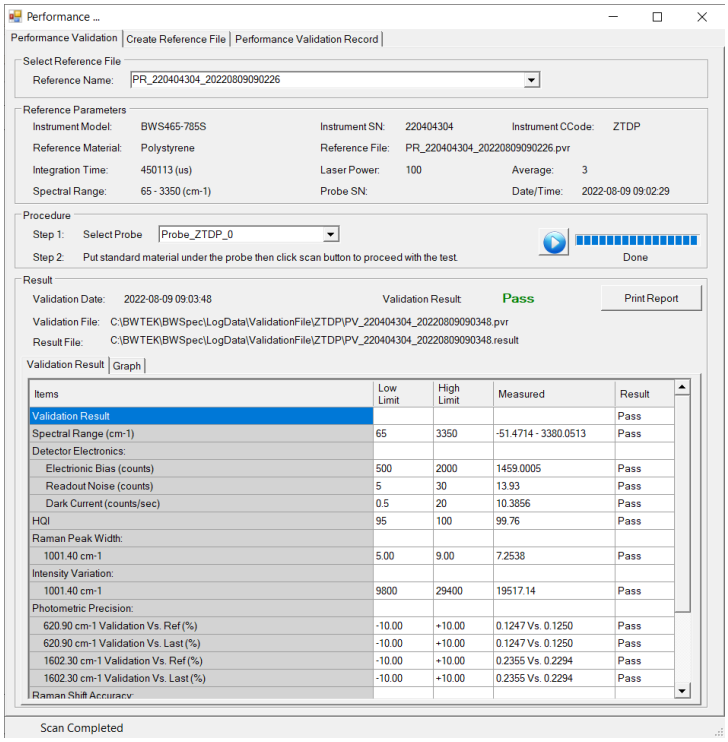
All parameters are set to default values but can be changed.

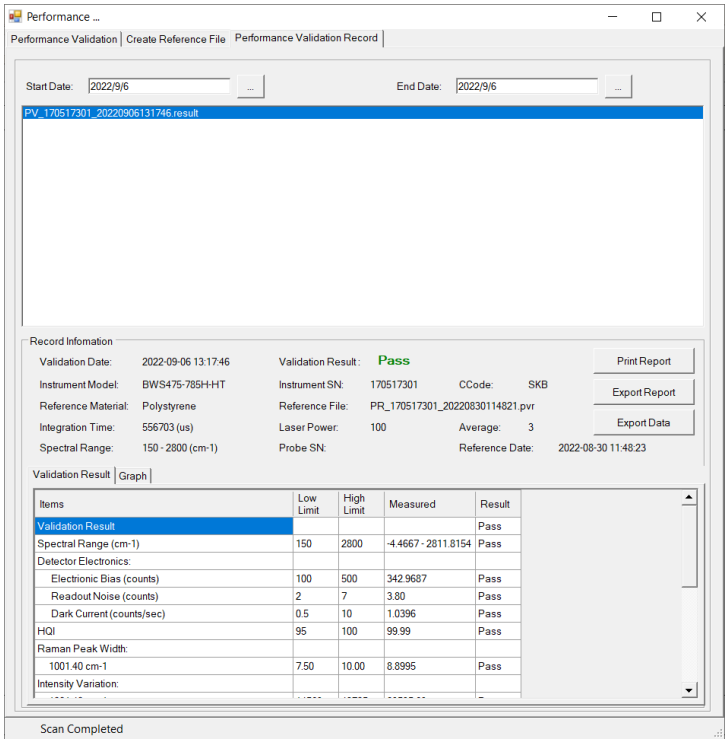
When the Performance Precheck box is checked, Dark1, Dark2, and Dark(60s) scans will be taken. If unchecked, these dark scans will be skipped to shorten the time to complete PVR file creation.

Performance Validation

After a PVR file has been created, Performance Validation can be run. Under Reference Name, select the PVR file to validate against. Select the connected probe from the Select Probe menu, then ensure the reference material is the same as what was used to create the PVR file. Press the blue play button to begin the Performance Validation. When complete, Pass/Fail results will appear in the Result section.

The Performance Validation report can be printed.





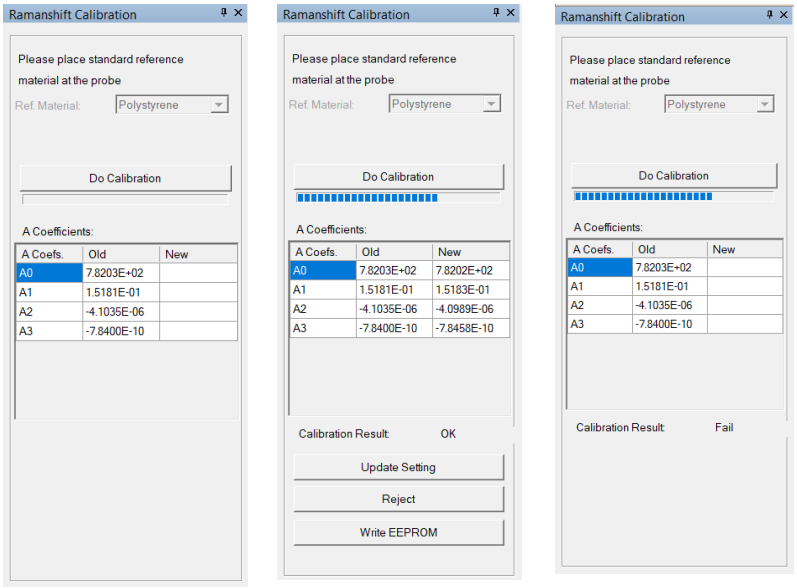
Performance Validation Record

Previously completed Performance Validation records are saved and viewable here. Records are displayed according to the Date range selected. To view the results, click the name of the *.result file to be viewed. The report can be printed or exported as a .txt file, or the data can be exported as a .txt file.

Raman Shift Calibration

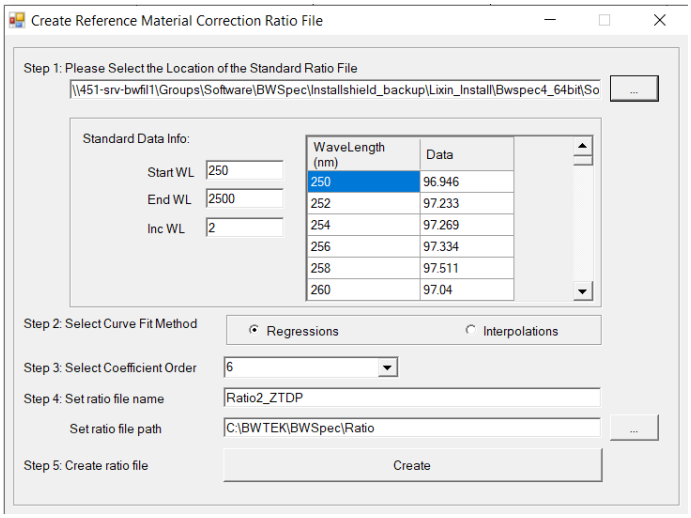
Raman shift calibration is performed when a performance test fails due to one or more peak positions are out of spec. A standard ASTM certified material Polystyrene is required for this calibration.

When this calibration is done successfully, user can choose to save or reject. User can then click Update Setting to update local A-coefficient settings, Reject to reject the calibration result or Write EEPROM to update A-coefficient in the device EEPROM.



Reference Material Correction

Click  and browse to locate the “Reference Material ratio.txt” file. The default path is: 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.

Relative Intensity Correction

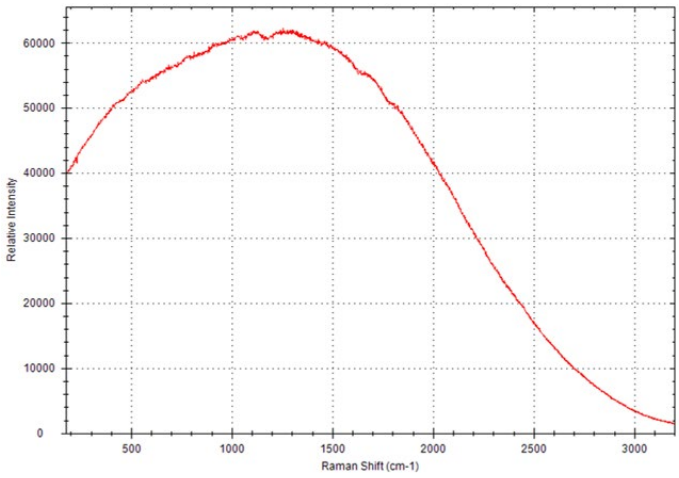
Relative Intensity Correction...

This calibration comes standard with B&W Tek's Raman systems.

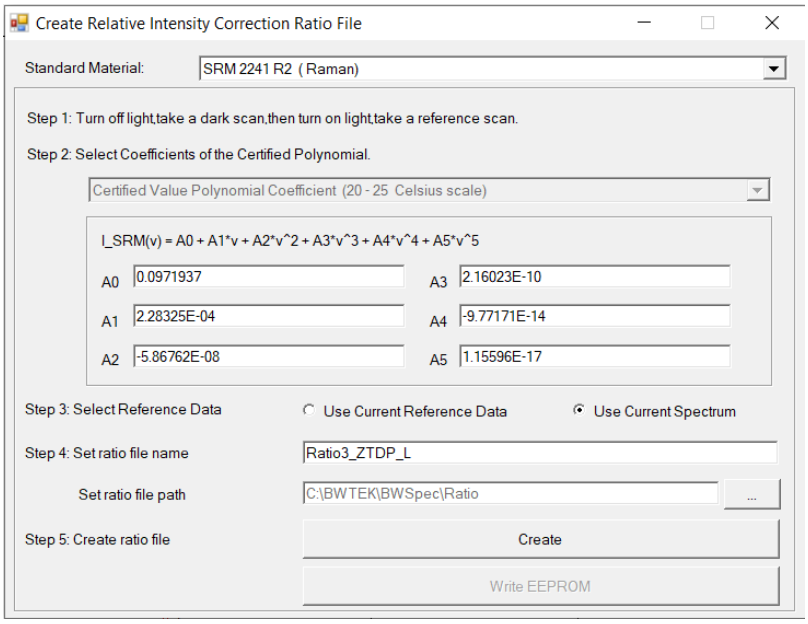
Determine the appropriate integration time: use the standard reference material SRM2241 (for 785nm), SRM2242a (for 532nm) or SRM 2244 (for 1064nm) to run a scan. The integration time of the scan should be adjusted to a value such that the highest intensity level is just below saturation level (65000 counts).

Run a dark scan with the same integration time. For B&W Tek 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.



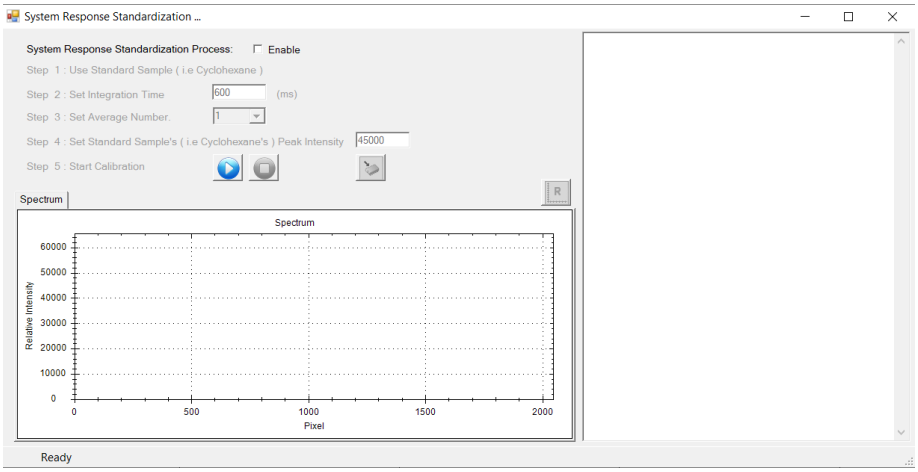
From the Menu Bar, select Tools > Relative Intensity Correction. The Relative Intensity Correction window will appear.



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.

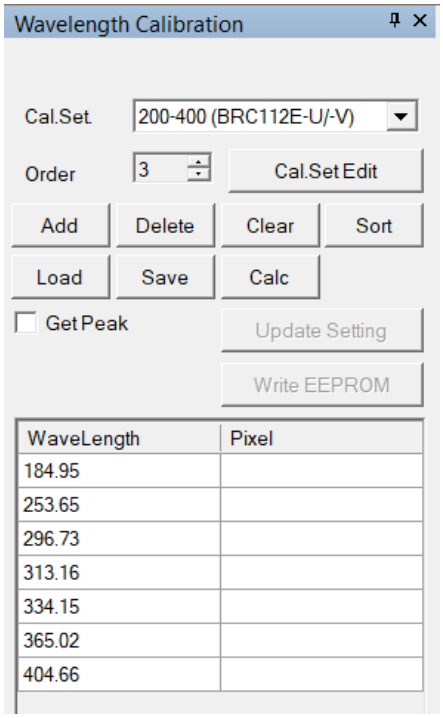
System Response Standardization

Previously named "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, certified Service Center, or Distributor equipped with specialized calibration setups. B&W Tek will not be responsible for any loss of your work and for any consequence if factory configuration is accidentally changed or corrupted.

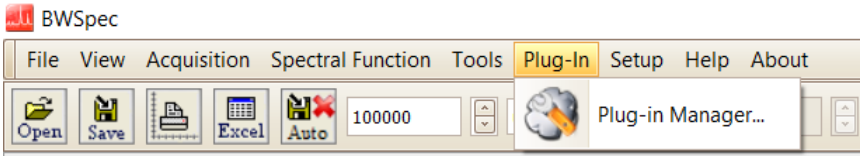


Wavelength Calibration

This function is not intended to be used by end users. If your spectrometer needs calibration, please contact B&W Tek at www.bwtek.com. Wavelength Calibration must be conducted by B&W Tek, Distributors, or OEM customers equipped with certified and traceable Light Standards and specialized calibration setups.

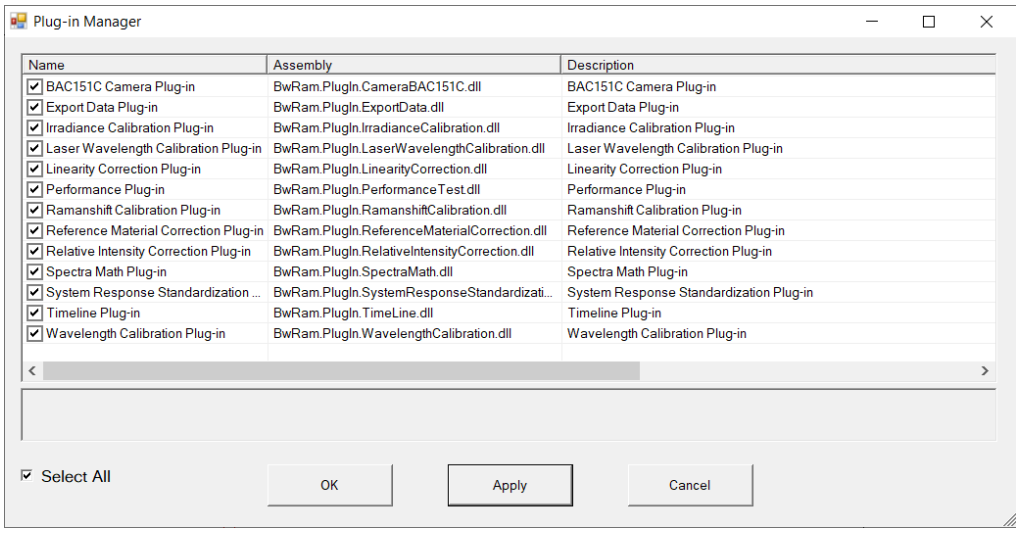


11 PLUG-IN

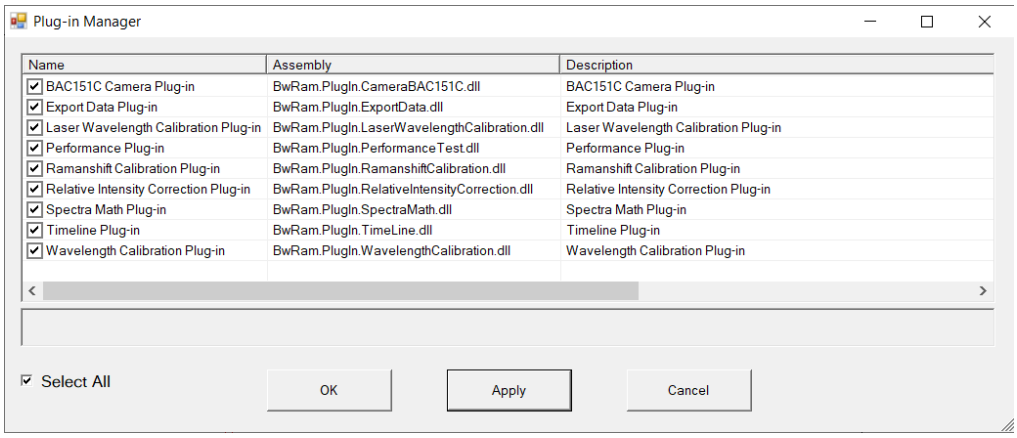


Opens the **Plug-In** window, listing all the available software Plug-Ins.
Check the box next to a given Plug-In to activate it. Click **Apply** and then **OK** to activate the Plug-In in the BWSpec Menu Bar. The Plug-Ins will be added to the appropriate menu on the BWSpec Menu Bar. The available Plug-ins depend on which workspace the user has selected.

BWSpec:



Raman:

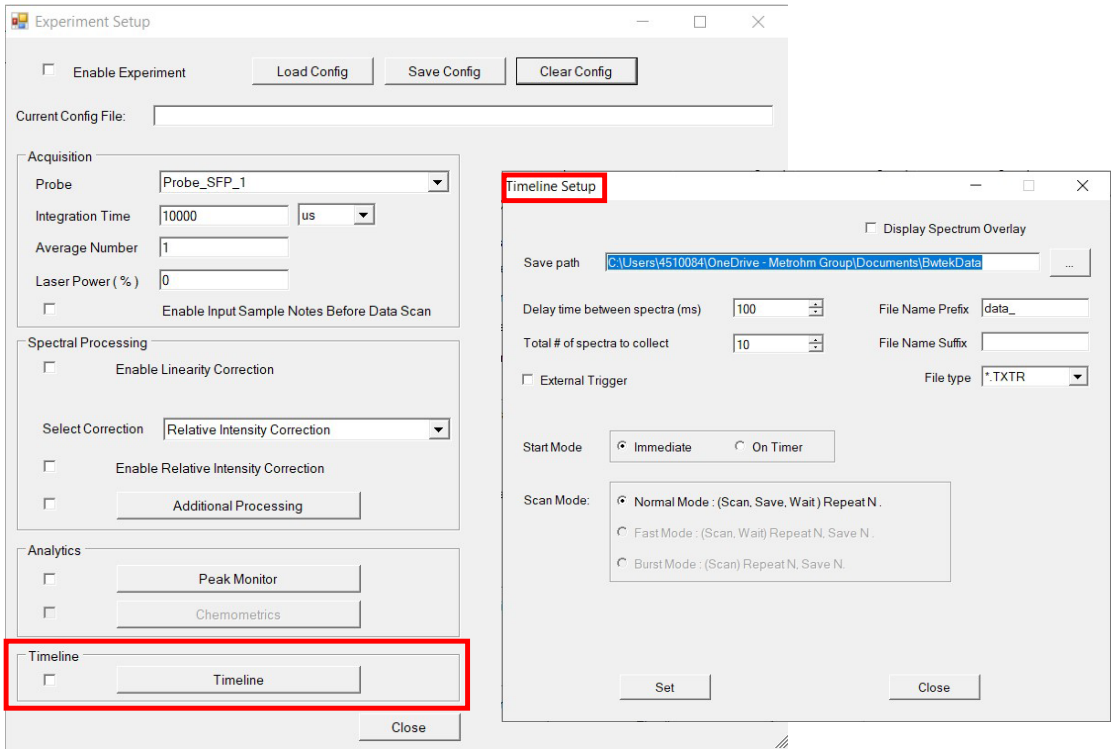


Timeline Plug-in

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

If Dark and Reference spectra are taken before beginning timeline, they will be added to all additional timeline created spectra.

Location: Menu Bar → Setup → Experiment Setup



Enter settings, including interval time (the delay time between each spectral acquisition), number of scans, file name suffix and/or file name prefix, data format for saved files and save path.

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.

When using Timeline, the regular Acquisition and Continuous Acquisition buttons are greyed out and replaced with the Timeline Acquisition button.

The Main Graph will split into a Dual chart. The top graph will display the current Raw data and any overlay data. The bottom Chart will display Peak Monitoring as a function of time.

Note:

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

Timeline Load

This function allows user to re-run previously saved Timeline series with the ability to re-define data processing and analysis.

To automatically load the files that were saved previously, click File and select 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.

May be used with Batch Re-Process to reprocess the data as you load it into BWSpec.

Note: Any configuration file created in Batch Process may not be cross compatible with this function. It is recommended to create a new configuration file for each mode if both modes are to be used

To perform analysis and display results in lower chart, check Batch Process Setup and define the data processing steps and analytics as in Experiment Setup. For convenience, some settings can be copied from the current Experiment Setup and then edited.

Location: Menu Bar → File

Click the  button to automatically load each data file from the folder into the Spectrum List panel sequentially. If **Batch Re-Process Setup** is checked, each loaded spectrum will have the Batch Re-Process applied

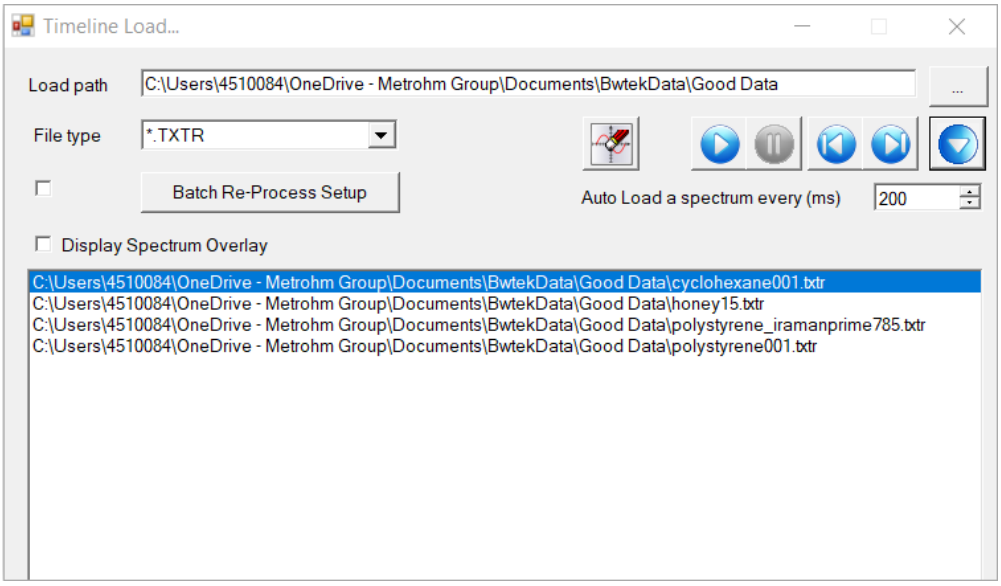
Click the  button to manually load the spectrum file forward, one at a time.

Click the  button to manually load the spectrum file backwards, one at a time.

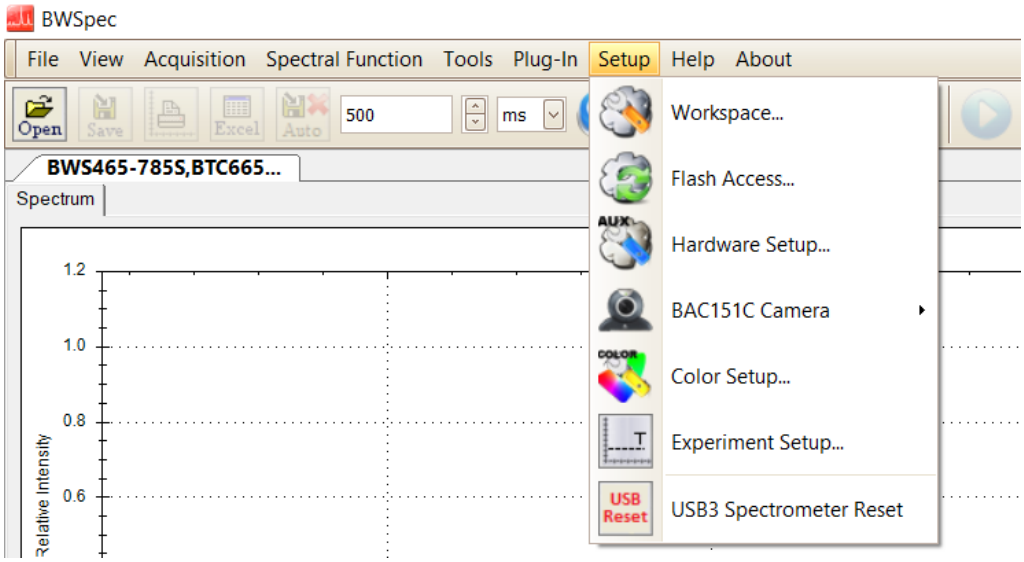
Click the  button to resize the Timeline Load window.

Click **File type** to select a saved file format.

Display Spectrum Overlay shows each loaded spectrum in the chart together instead of one at a time.

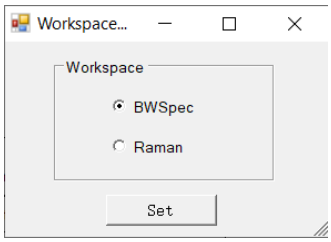


12 SETUP



Workspace

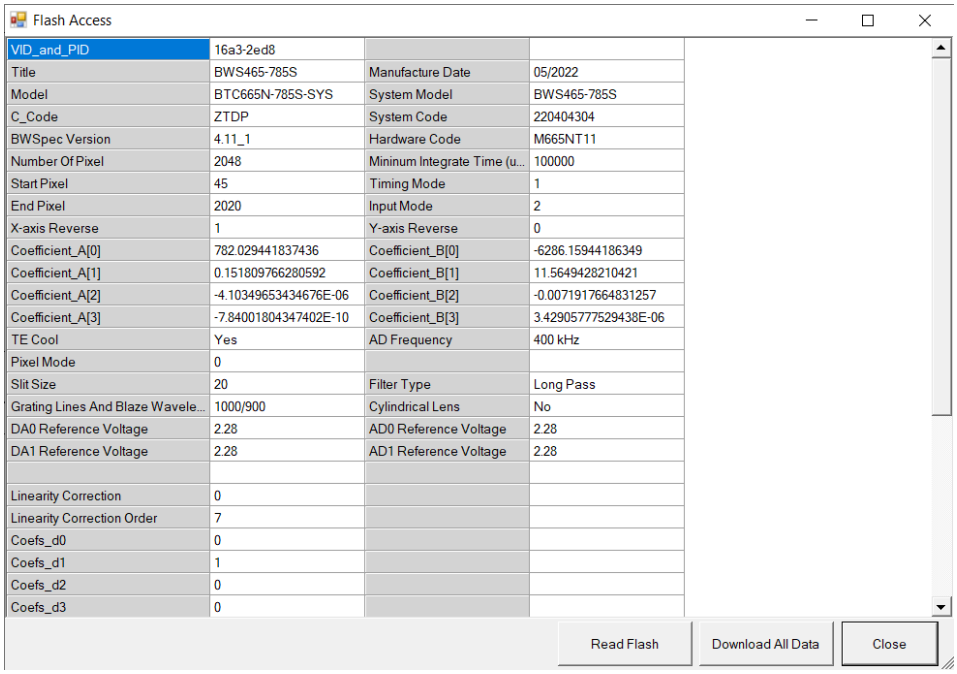
The Workspace Setup window allows switching between the BWSpec and Raman workspaces.
The Raman Workspace has configurations and rules tailored for Raman applications in the Spectrometer Control Panel.



Flash Access…

The Flash Access window provides unique information pertaining to the defaults and settings of the spectrometer.

Clicking the **Read Flash** button reads the spectrometer's EEPROM (device memory) and resets the BWSpec variables back to their default factory values which include wavelength calibration, display scales, and linearity correction.

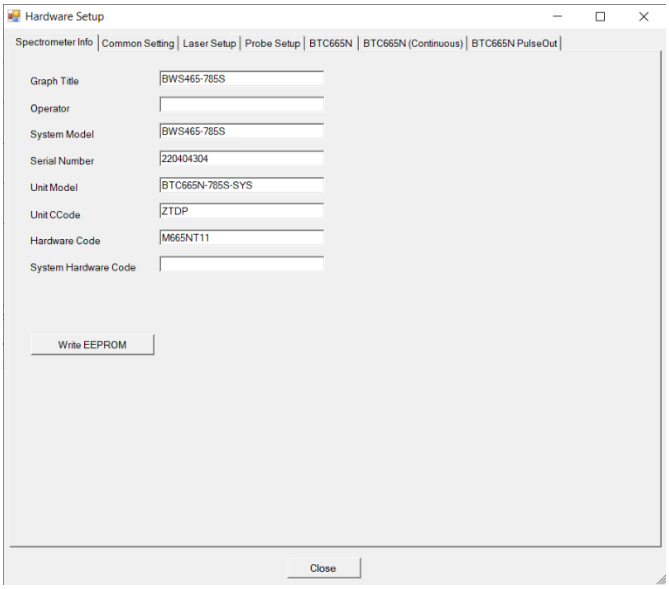


VID_and_PID	16a3-2ed8		
Title	BWS465-785S	Manufacture Date	05/2022
Model	BTC665N-785S-SYS	System Model	BWS465-785S
C_Code	ZTDP	System Code	220404304
BWSpec Version	4.11_1	Hardware Code	M665NT11
Number Of Pixel	2048	Mininum Integrate Time (u...	100000
Start Pixel	45	Timing Mode	1
End Pixel	2020	Input Mode	2
X-axis Reverse	1	Y-axis Reverse	0
Coefficient_A[0]	782.029441837436	Coefficient_B[0]	-6286.15944186349
Coefficient_A[1]	0.151809766280592	Coefficient_B[1]	11.5649428210421
Coefficient_A[2]	-4.10349653434676E-06	Coefficient_B[2]	-0.0071917664831257
Coefficient_A[3]	-7.84001804347402E-10	Coefficient_B[3]	3.42905777529438E-06
TE Cool	Yes	AD Frequency	400 kHz
Pixel Mode	0		
Slit Size	20	Filter Type	Long Pass
Grating Lines And Blaze Wavele...	1000/900	Cylindrical Lens	No
DA0 Reference Voltage	2.28	AD0 Reference Voltage	2.28
DA1 Reference Voltage	2.28	AD1 Reference Voltage	2.28
Linearity Correction	0		
Linearity Correction Order	7		
Coefs_d0	0		
Coefs_d1	1		
Coefs_d2	0		
Coefs_d3	0		

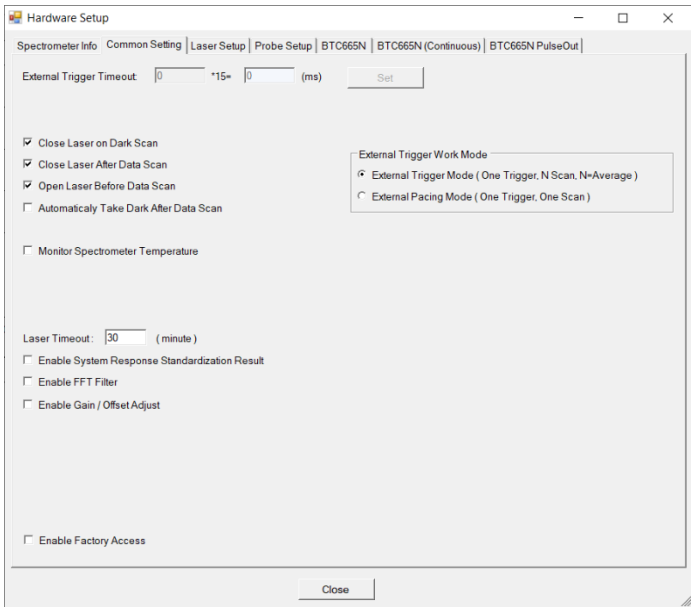
Hardware Setup

This menu is active only when status is online.
Not all features in this manual are applicable to any spectrometer. Check product's user manual for details.

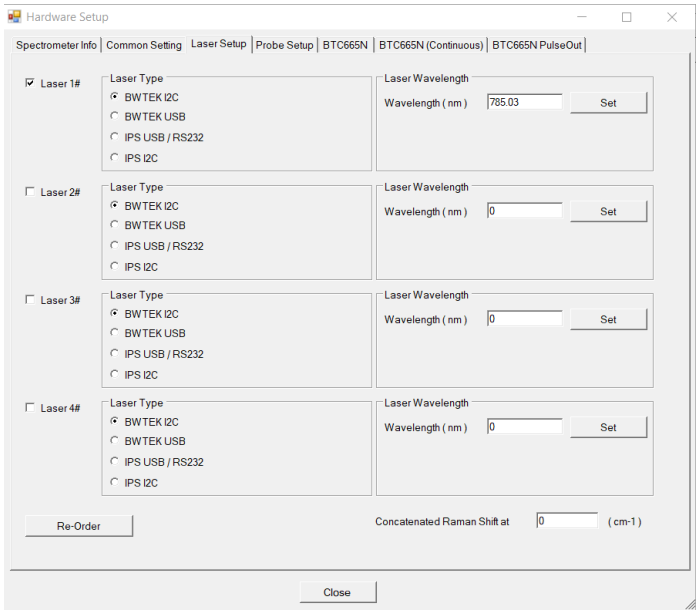
- Spectrometer info:
  This is to display spectrometer info of the online instrument. Values can be revised and saved to EEPROM with password.



- Common Setting:



- Laser Setup:



- Probe Setup:

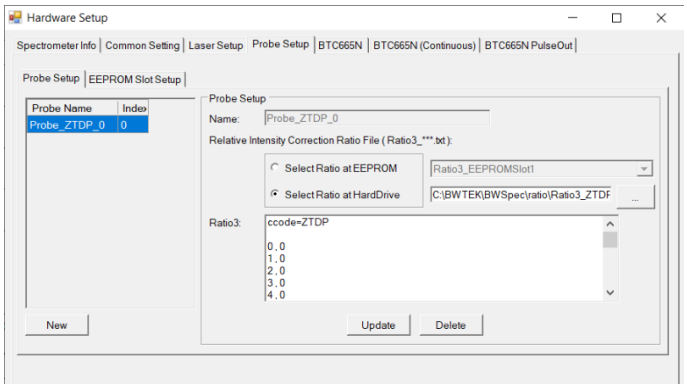
The **Probe Setup Tab** is to pre-configure probes for the system and defines which Raman Probe is available in the Experiment Setup.

Select the Relative Intensity Correction ratio file provided on the BWSpec Installation flash drive. If you are missing your Ratio3 file, you may request a copy by contacting us at www.bwtek.com

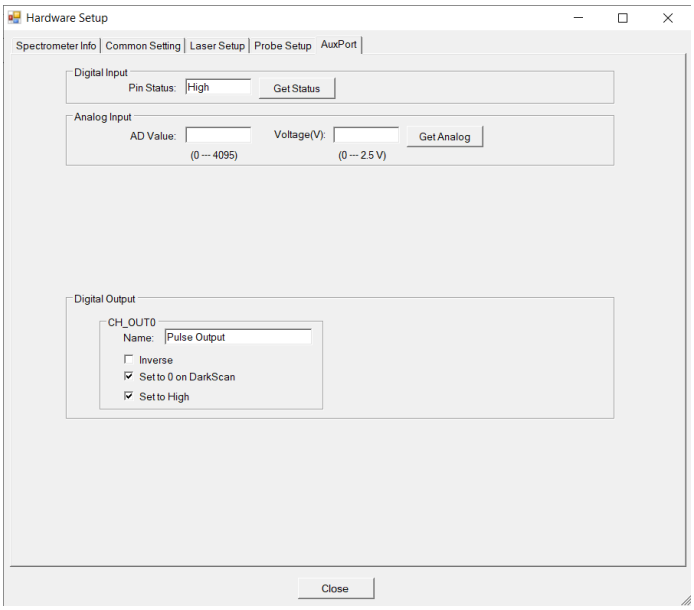
The Ratio3 information will now be displayed, Click **Done** to accept.

You may use the Ratio3 created at the factory or you can create your own. Experienced customers can refer to the Relative Intensity Correction section for more details. The appropriate Standard Reference Material is required to create a good Ratio3 correction file.

EEPROM Slot Setup: Do not use this feature.

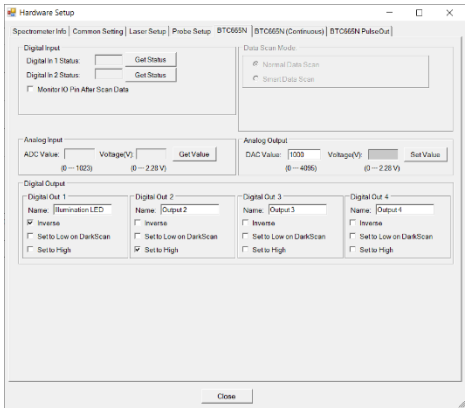


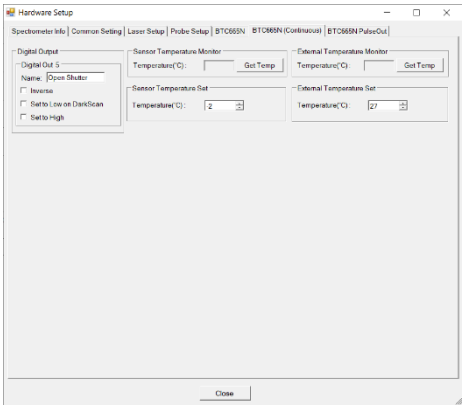
- Aux Port:

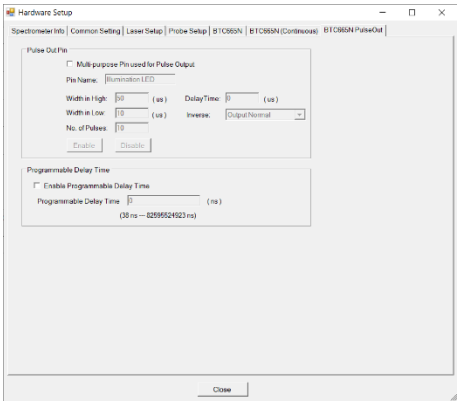


Spectrometer configuration:

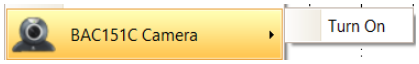
Optional configurations for different hardware types. Check product user manuals for operation details.





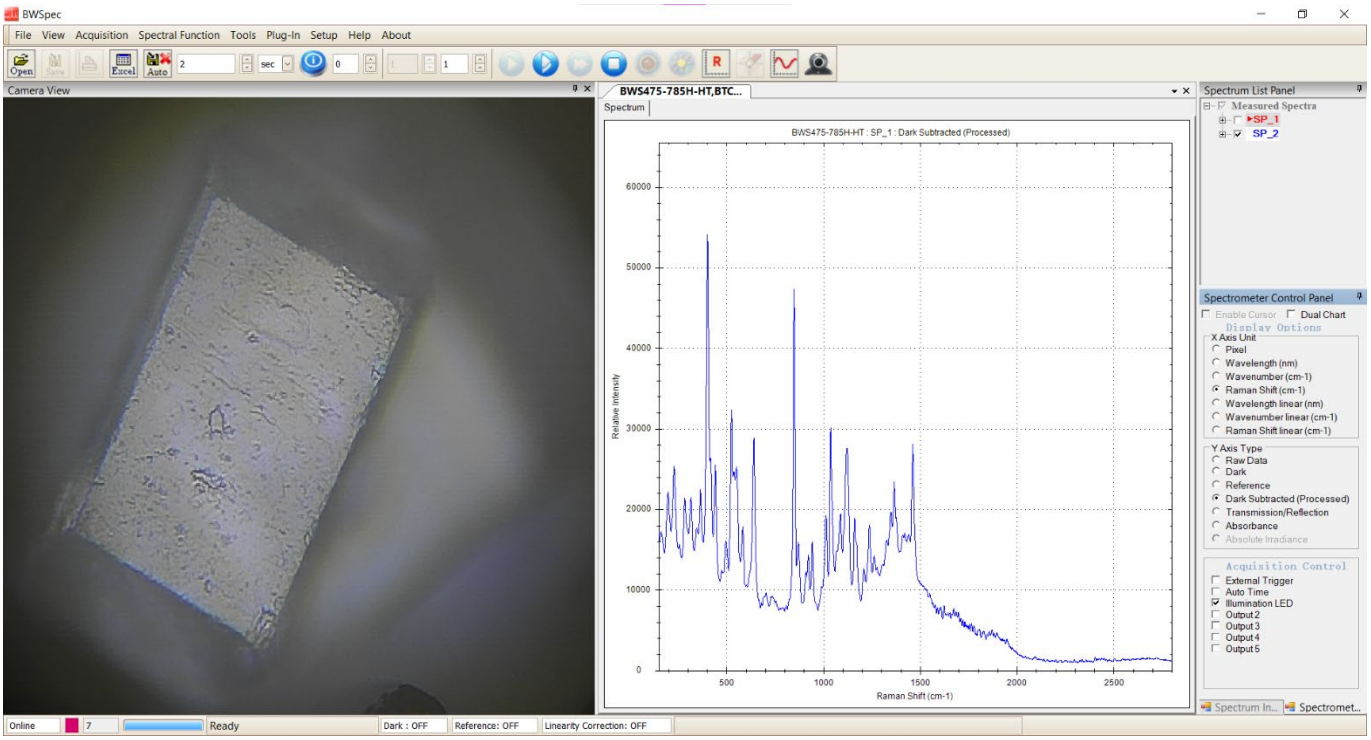


BAC151C Camera



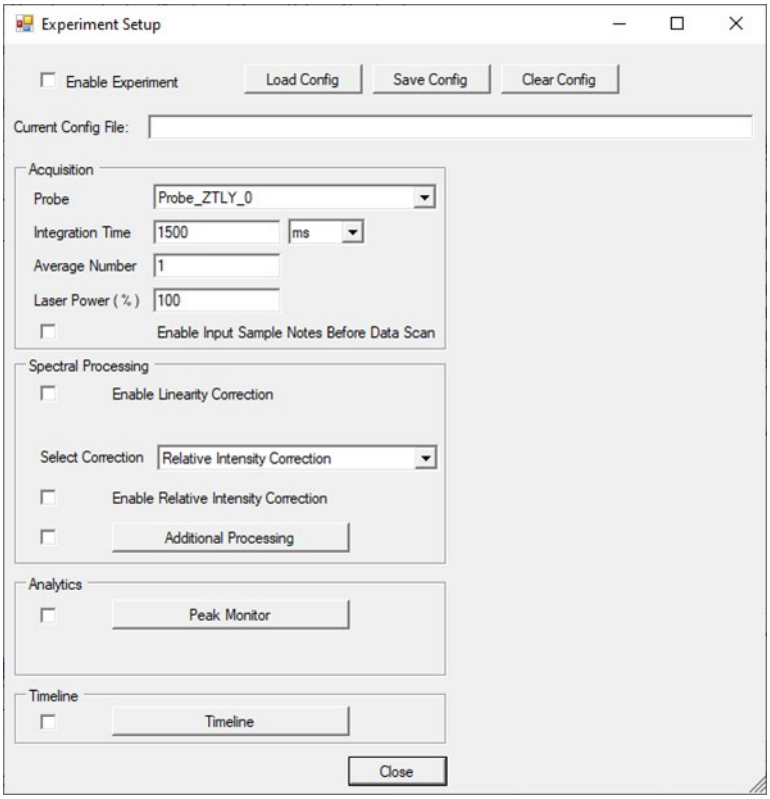
Turns on the BAC151C camera

Refer to the BAC151C User Manual for details on installation and use.



Experiment Setup

Experiment Setup can be viewed from the Raman Workspace:



Allows the user to create and save a set of parameters to define how data is collected and saved. This includes Acquisition, Spectral Processing, Analytics, and Timeline.

Load Config loads a previously saved Experiment Setup.

Save Config saves the current Experiment Setup. Changes made to the current setup are lost unless they are saved.

Clear Config deselects the Enable Experiment box and resets any selections in the Experiment window.

Current Config. File is highlighted yellow if any change is made and has not been saved.

Changes made to the parameters are applied when the new configuration is saved; the acquisition parameters shown in other places will change accordingly.

These Spectral Processing and Analytics are applied to Dark Subtracted (Processed) Data.

There is checkbox to enable/disable Experiment. When it is checked, all setting parameters defined in Spectral Function will be overwritten by those from loaded Experiment config file unless not

defined there.

Acquisition:
Define the settings the instrument will use in each acquisition; including integration time, number of averages used for all instruments, laser power and probe used for Raman.
A probe can be easily selected from a list of probes pre-configured in Setup=> Hardware Setup=> Probe Setup.
For Raman instruments, a **Probe** must first be enabled/selected to enable Spectral Processing. Refer to the Hardware Setup section for more information on Probe Setup.

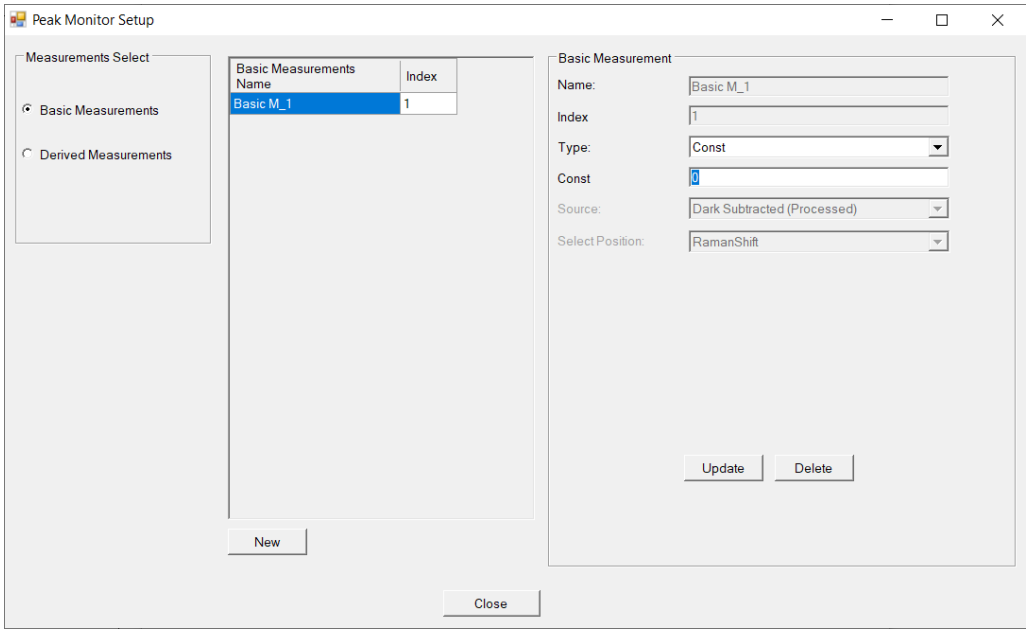
Spectral Processing:
This section is used to define which data processing should be performed.
Options for intensity correction include: Linearity Correction, Irradiance Calibration, Reference Material Correction, and Relative Intensity Correction.
Relative Intensity Correction is the only option available in the Raman workspace.
When Dark Subtraction is enabled, it is performed prior to any Spectral Professing listed here.
Irradiance Calibration and Reference Material Correction require a ratio file created by the factory. Relative Intensity Correction also requires a ratio file, but it is defined in Hardware Setup/ Probe Setup.
Dark Subtraction should be used with Raman instruments; Relative Intensity Correction cannot be applied unless Dark Subtraction is done first.
Additional Processing allows for multiple post processing steps to be applied after the intensity correction. This includes **Baseline Removal**, **Smoothing**, and **Derivative**. These functions are also available in Spectral Functions for post-measurement processing; refer to Section 9 for more details.

Analytics
This menu provides spectral analysis functions to be performed on the Processed Data block.
The results are displayed in the Analytics tab which appears on the main form.
The Peak Monitor allows the user to perform peak analysis on automatically defined peaks, and do arithmetic on the analysis results
To define Measurements variables, select Basic Measurements or Derived Measurements.

Basic Measurements…

Define the peaks property values

Press the New button to add a new Measurement variable.



The **Name** is to distinguish this measurement; this will be the title in Analytics.

The **Index** will start at 0 and automatically increase for each additional measurement.

The **Type** defines which peak parameter is being measured; Refer to Appendix C for a description and visual representation of Peak Property Values. Note BWSpec workspace shows all types available, while Raman only focuses on Raman specific types.

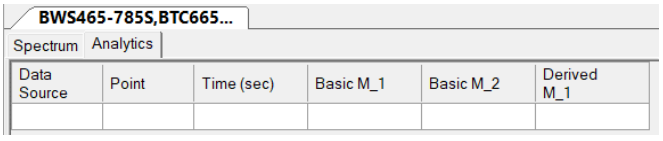
The **Source** is always Dark Subtracted (Processed Data) in Raman workspace. You can also select %T/R, Absorbance, or Absolute Irradiance in BWSpec workspace

Select Position specifies the x-axis unit used to select the peak: Pixel, Wavelength, or Raman Shift.

Start and End - the highest peak found within the range defined by these two values will be taken as the peak.

Delete: press this to delete the selected variable. A variable cannot be deleted if it is used to define one or more Derived Measurements. All such Derived Measurement variables must be deleted first.

After the Experiment Setup is saved, the Analytics tab will appear in the top left of the main graph, where the measurements are displayed in a table.



Derived Measurements…

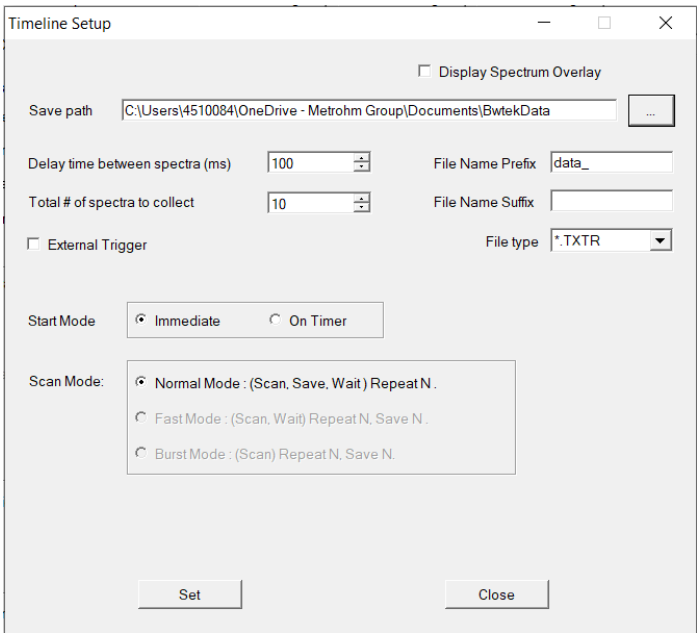
Define measurement variables that are derived from the Basic Measurements. Press the New button to add a new Measurement.

The **Name** to identify this measurement; this name will be the title in Analytics.

The **Index** will start at 0 and automatically increase for each additional measurement.
The **Operation** defines the type of math operation to be applied using Measurement A and/or B.
The **Measurement Type** is chosen between Constant, Basic Measurement and Derived Measurement.
For example, to measure the peak height ratio of peak A and Peak B, first define two Basic Measurement variables representing heights of peak A and B, then define a Derived Measurement variable as A/B.

Timeline

To perform kinetic measurements and analysis.
Enable this function in the Plug-In Manager.
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 and are displayed individually in the main graph.
If Dark and Reference spectra are taken before beginning timeline, they will be added to all additional timeline created spectra.
Enter settings, including interval time (the delay time between each spectral acquisition), number of scans, file name suffix and/or file name prefix, data format for saved files and save path.
The spectra collected will be saved in the designated path. If no specific suffix is assigned, a default of _1, _2, _3, etc. will be assigned to each spectrum.
Refer to Section Timeline Plug-in for more details.



Raman Instrument Experiment setup example:

Find and measure multiple peaks using a Probe, Relative Intensity Correction and Additional Processing.

First, we are going to open Hardware Setup and setup the Probe information with the Relative Intensity Correction Ratio file. Then, we use that information in Experiment Setup and create an experiment to measure a Tylenol Tablet, apply baseline correction and smoothing, and find and measure a specific peak over time.

Probe Setup

Navigate to Setup => Hardware Setup and select the **Probe Setup** tab.

Click the **New** button, and Probe Setup will appear.

Enter an unique name for the probe, we recommend Probe_[Serial number of probe]_[Ccode of unit]; for example: **Probe_160216952_RJX**. This allows for a simple way to pair probes to instruments, especially if you have multiple probes.

Select the radio button Select Ratio at Hard Drive and click the **…** button.

Locate the Ratio3_[Ccode of unit].txt file, provided for you on the B&W Tek flash drive; for example; **Ratio3_RJX.txt**.

The Ratio3 information will now be displayed, Click **Done.**

Experiment Setup: Acquisition

Navigate to Setup => Experiment Setup

Under the **Acquisition** Section, in **Probe,** select the newly created Probe Profile; Probe_160216952_RJX.

Select an **Integration Time** and unit suitable for your substance. You can determine optimal integration times by collecting data in the main window that gives the best spectrum for your sample; where the peaks of interest are at about 50,000 counts.

Select an **Average Number**, 1 is typical, but more may be needed if you have longer integration times or low Signal to Noise Ratio (too much noise).

Select a **Laser Power %** to use; 100% is good for white or light colored samples. Colored samples may use 60% and Dark colored samples may use 10-20% or lower. If you burn the sample, use a lower laser power and a longer integration time.

Experiment Setup: Spectral Processing

Under the Spectral Processing Section, Select the Correction Relative Intensity Correction.

Check the box next to Enable Relative Intensity Correction.

Check the box next to **Additional Processing**, and then click the button to open the Post Processing Setup window.

Click **New** to add a Data Process. In our example we are going to do smoothing,

Under **Name** we type in **Smoothing**, in **Type** we select **Smooth**, and under **Smoothing Type** we select **Savitzky-Golay Smoothing** with a window size of **2**. Then click the **Done** button to add this Data Processing. Click **Close** to exit the window.

Experiment Setup: Analytics

Check the box next to **Peak Monitor**, and then click the button to open the Peak Monitor Setup window.

Click **New** to add a Basic Measurement. In our example we are going to measure the Tylenol peak height above the baseline at ~1324 Raman shift

Under **Name** we type in **Peak 1324**, in **Type** we select **Peak Height**, and under **Select Position** we select **RamanShift** with a Start and End of **1314** and **1334** respectively. Then click the **Done** button to add this to Basic Measurements. Click **Close** to exit the window.

Experiment Setup: Timeline

Check the box next to **Timeline**, and then click the button to open the Timeline Setup window.

Check the box **Display Spectrum Overlay** to have all the timeline acquisitions display in the main graph.

Click the **…** to select a save location for the new data.

Select the **Delay time between spectra (ms)**, in this example we select **0**.

Select the **Total # of spectra to collect**, in this example we select **12**.

Click **Set** to accept the Timeline settings.

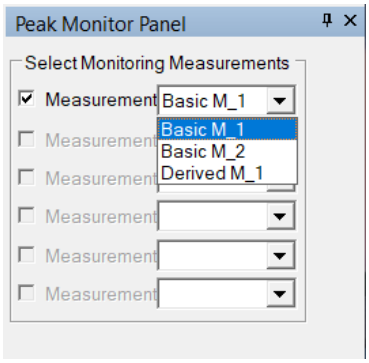
Experiment Setup

Click the **Save Config** button and save the experiment setup configuration to a .cfg file.

Click the **Close** button at the bottom to close the Experiment Setup window. The main graph will adjust and display a dual chart for timeline, along with the Timeline Acquisition button and Analytics tab.

Using the Experiment

Click the Timeline Acquisition button  to begin taking data.



The top graph will display each spectrum as an overlay.

The bottom graph will display the Peak Monitoring (Peak Height in this case) as a function of time. To toggle different peaks, go to the Peak Monitor Panel at the bottom right and select the peak from the dropdown menu to activate the Measurement.

At the top of the main graph the Analytics tab will record the Peak Height for each scan.

To exit Timeline mode, go back to Experiment Setup and uncheck the Timeline box. Alternatively, you can go to Setup > Flash Access > Read Flash.

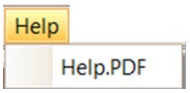
USB3 Spectrometer Reset

USB3 Spectrometer Reset

This button is only available for USB 3.0 units such as the Exemplar series, i-Raman Plus, and i-Raman Pro.

Performs a “Hardware reset” of the USB connection. This is functionally the same as unplugging and plugging back in the USB cable.

13 HELP

Opens the BWSpec User Manual as a .PDF document. 

This .PDF is also available in the BWSpec installation folder location (C:\BWTEK\BWSpec).

14 ABOUT

The **About** window provides B&W Tek contact information BWSpec software version number.

15 TOOLBAR

Open 

Refer to function in menu File->Open Spectrum…

Save 

Refer to function in menu File->Save Selected Spectrum…

Print 

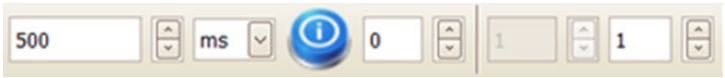
Refer to function in menu File->Print...

Excel 

Refer to function in menu File->Excel

Auto Save 

This is to enable/disable auto saving on scanned data

Integration Time Control 

Total Integration Time = Integration Time * Multiplier

For Set Integration Time: Maximum Value is based on the Time Unit while minimum Value is based on the capability of the detector. Refer to product user manual for details.

Unit

Time unit for spectrometer acquisition time.

Set to minutes (min), seconds (sec), milliseconds (ms), or microseconds (µs). Some units are not available in Raman workspace.

Time Average

Range 1 – 65535.

Average value will take the time average multiplied by the number of scans at the given total 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 ratio.

Acquire Control

Refer to Section 8 **Acquire** for more information.

Reset Graph

Reset the graph to the default X-axis range for the spectrum and the Y-axis to the set scale. The set scale may be changed in

Display Scales.

Clear Display 

Remove all spectra from the **Spectrum List Panel** and display area.
The same function as menu File->View->Clear All Spectral Data…

Display Scales 

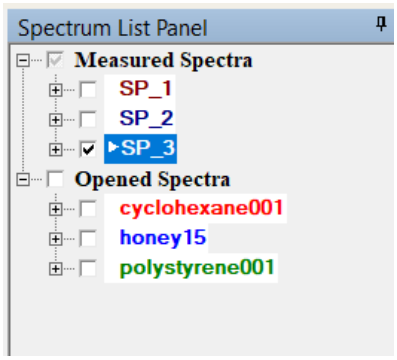
Opens the **Display Scales** Settings window.
The same function as menu File->View->Display Scales…

BAC151C Control 

Turns on the BAC151C Camera and opens a new View Window.
The BAC151C Plug-in must be enabled in Plug-In Manager.
Refer to the BAC151x User Manual for further details.
Enables manual control of LED Illumination through checkbox under Acquire Control.
Enables automatic control of LED Illumination during scans.
If LED is on before any scan, the LED will turn off automatically during the scan, then back on when completed.
If LED is off before any scan, the LED will stay off until manually turned back on.
Enables the BAC151x button in Toolbar.
Location: in the Menu Bar → Setup
Refer to the BAC151x User Manual for details.
Note: Disable this Plug-in to properly use spectrometers with built-in shutters.

16 SPECTRUM LIST PANEL

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



Spectra listed are classified into two categories. The Measured Spectra refer to those acquired from an instrument, and Opened Spectra are those loaded from a folder. Measured spectra are numbered sequentially with a prefix “SP_”.

Spectra with checkmark ☑ are “Checked” spectra and are displayed in the graph. Spectra without the check marks are hidden from the current graph display.

The spectrum highlighted with ▶ arrow (color may vary) next to its name indicates the spectrum currently selected. There can only be one Selected spectrum at a time.

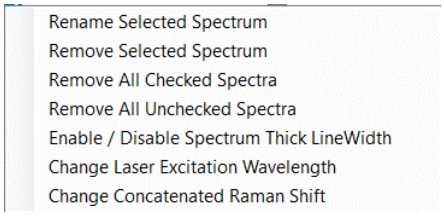
The “active” spectrum will have the current data overwritten if additional spectra are taken.

A dark spectrum is used to subtract the contribution of the sensor itself. This is carried over until a new dark spectrum is acquired.

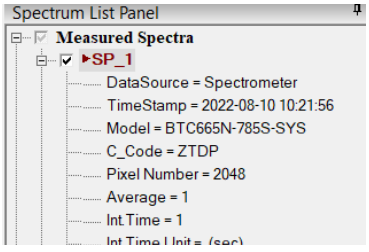
To ensure data integrity, BWSpec prevents the measurement of a new spectrum when the last measured spectrum is unfinished, such as, when in Raman Workspace, the integration time of the signal and the dark spectrum are not the same. If the last Measured Spectrum has a raw and dark with different integration times, and an overlay is attempted, BWSpec will alert the user that the integration time of the raw and dark do not match.

If the last Measured Spectrum is unfinished and is selected, it can be overwritten by a new measurement. No other spectrum can be overwritten by a new measurement.

Right Click on individual spectrum from the list will bring up the following menu on the right→:

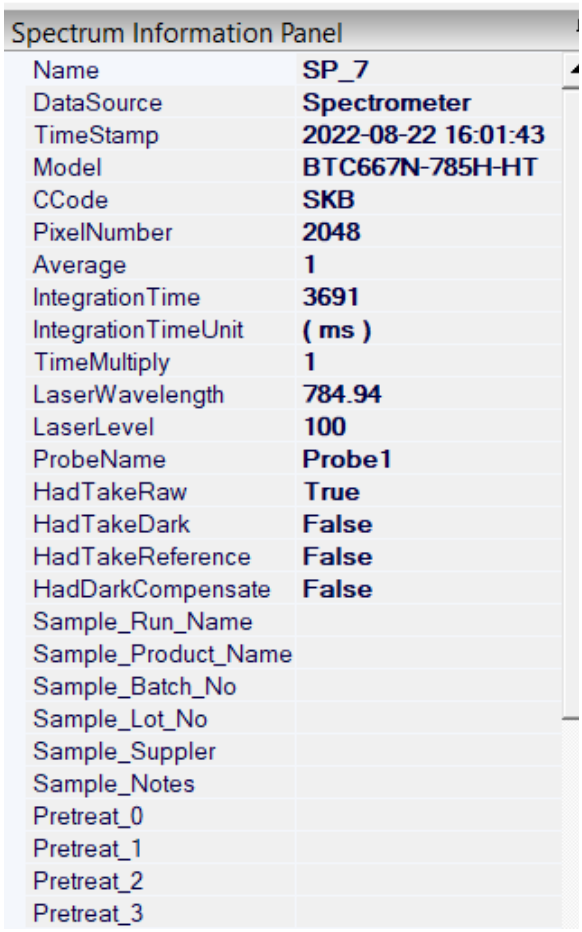


Toggle the + sign to expand the information for a spectrum like below ↓:



17 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.
Below is a short description of each entry:



Name: Name of the spectrum in the Spectrum List Panel.

DataSource: Spectrometer or Load File

Model: Model Number.

CCode: Configuration Code, related to Serial Number.

PixelNumber: Number of pixels in detector.

Average, Integration Time, Integration Time Unit; Details from the Toolbar.

Laser Wavelength: For Raman only, otherwise set to default 785

Laser Level: Laser Percentage from the Toolbar.

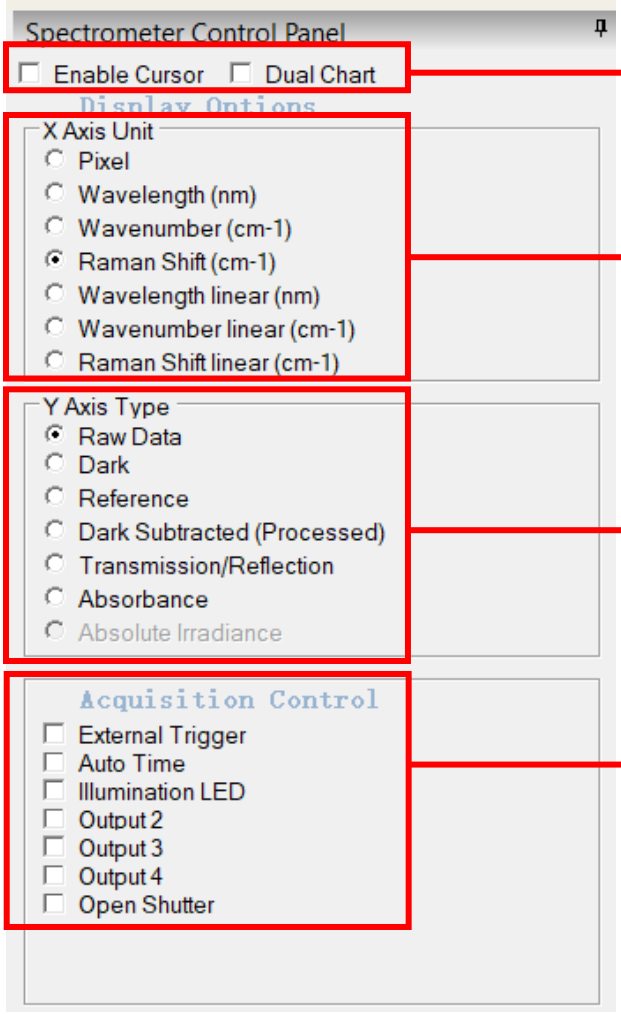
Probe Name: For Raman only, from Hardware Setup.

HadTakeRaw, **HadTakeDark**, **HadTakeReference**: True or False depending on if the acquisitions are taken.

Pretreat_X: Data processing (smoothing, baseline removal, derivative, spectral math) steps for the Processed Data block are saved here.

18 SPECTROMETER CONTROL PANEL

The following sections are detailed descriptions of each item in the **Spectrometer Control Panel**.
Each Workspace has default options in the Spectrometer Control Panel. Below is shown for the **BWSpec Workspace**.



Additional display options

Select desired X-axis spectrum display mode.

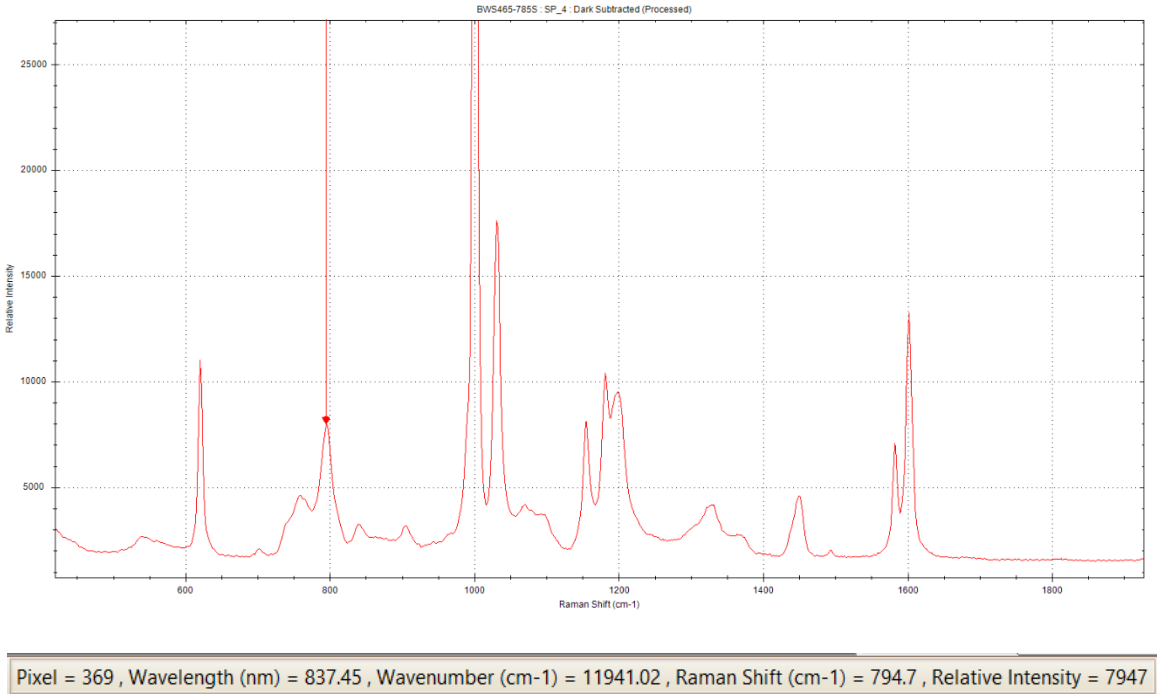
Select desired Y-axis spectrum display mode.

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

Enable Cursor

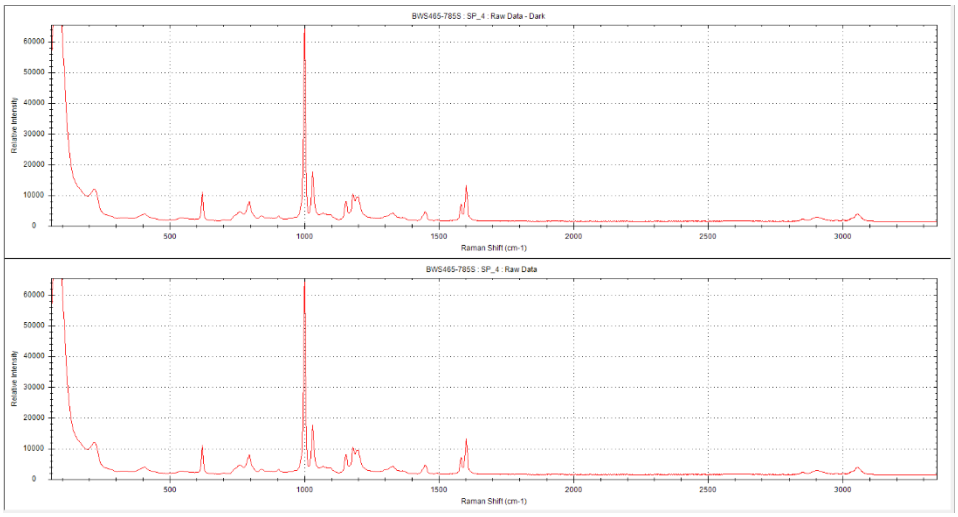
This provides a vertical line on the graph which follows the mouse cursor. Information relating to the cursor location on the graph will be displayed at the bottom of the window in the status bar.

This feature can only be used on a spectrum that is displayed on the graph while the instrument is not acquiring data.



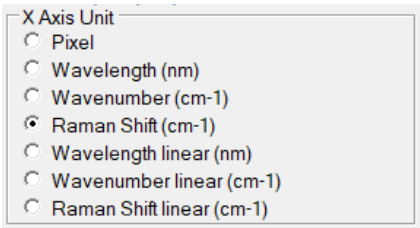
Dual Chart

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

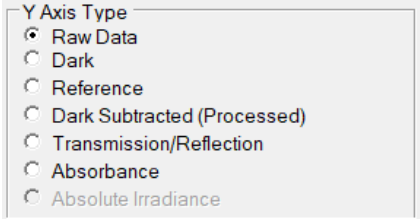


X Axis Unit

Changes the X-axis display mode.

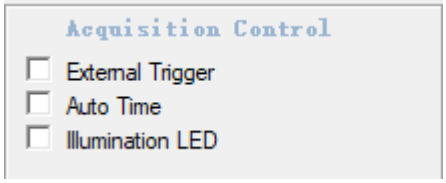


Y Axis Type



Changes the Y-axis display mode.
Raw Data: Shows raw form of the spectrum.
Dark: Shows the Dark Array spectrum.
Reference: Shows the Reference Array spectrum.
Dark Subtracted (Processed): Starts as (Raw – Dark) without any spectral processing. All additional spectral processing applies to this Y-Axis instead of Raw, Dark or Reference.
Transmission / Reflection (%): [(Raw– Dark) / (Reference– Dark)] * 100
Absorbance: -log (Transmission (%) / 100)
Absolute Irradiance: Shows the corrected spectrum when Irradiance Calibration is enabled.
The spectrometer must have a valid Irradiance Calibration file.
Refer to the Irradiance Calibration section for additional details.

Acquisition Control



External Trigger

When enabled, the external trigger will have the following two behaviors depending on the setting in 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 the Hardware Setup section and the product user manual for additional details.

Illumination LED

This option appears when any BAC151x Plug-In is enabled.

Manual control for LED illumination is available using the checkbox to toggle On/Off. LED Illumination will always automatically turn off during all Spectral Acquisition, including dark scan.

Auto Time

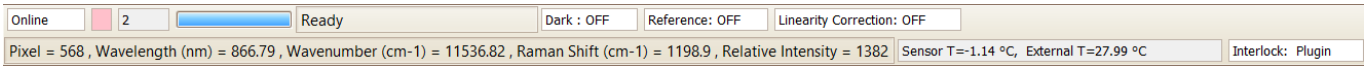
When enabled, the software will automatically scan and increase the integration time in increments until the response is close to saturation.

Once the scan is complete, Auto Time will be enabled until it is disabled manually.

This feature is meant to automatically find a suitable integration time for the given sample.

Note: Additional control options may also appear depending on your spectrometer or system. Refer to your Spectrometer's User Manual for more details.

19 STATUS BAR



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

Online / Offline 

Shows status of spectrometer.
Online – Spectrometer connected
Offline – Spectrometer not connected, check USB cable and Device Manager.

Scan count 

Increases in number with each scan.
The box color will change red to pink with each scan: → 

Acquisition status bar 

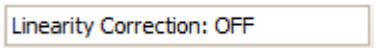
Increases as the scan progresses
Useful for long integration times or multiple averages.

Dark Array Status 

Gives status if a Dark Scan has been taken and saved into the Dark Array for the “active” spectrum.

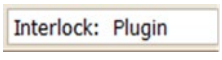
Reference Array Status 

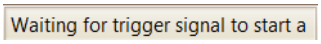
Gives status if a Reference Scan has been taken and saved into the Reference Array for the “active” spectrum.

Linearity Correction 

Gives status of the **Linear Correction** function

Temperature 

Interlock 

Trigger 

“Waiting for trigger signal to start acquisition” message (may be cut off).

Appendix A: Declaration of TXTR File

The TXTR (TXT Raman) 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 (highlighted by yellow). The flag block length may vary and an example of text file is shown below.

1. TXTR has extra data blocks to store the intensity correction ratio spectra (including Relative intensity correction ratio, Reference Material Correction Ratio, and Absolute Irradiance Correction Ratio). This ensures the integrity of spectral files and makes it easy to transport and reprocess them without loss of critical information.
2. TXTR added data processing audit trails to spectral file header to record the treatment steps for the Dark Subtracted (Processed Data) block starting from the Raw Data block. These are the numbered Pretreat lines and can be viewed in Spectrum List Panel.
3. Users are recommended to use this new file format.
4. File conversion utility can convert format between TXT and TXTR.

```
File Format;TXTR                    //File Format
File Description;TXT(Raman) file    //File Description
File Version;BWRam4.11              //File Version
Run Name;                           //Custom defined Run Name
Product Name;                       //Custom defined Product Name
Batch No;                           //Custom defined Batch Number
Lot No;                             //Custom defined Lot Number
Sample Supplier;                    //Custom defined Sample Supplier
Sample Notes;                       //Custom defined Sample Notes
Date;2017-05-24 01:22:41            //Date of File Creation
title;NNN                           //Spectrometer title name that saved data
model;BRC112-FIT11                  //Spectrometer model
c code;NNN                          //Spectrometer serial number
operator;                           //Operator that saved file
pixel_start;0                       //Sensor start pixel
pixel_end;2047                      //Sensor end pixel
units;3                             //X-axis unit (0=Pixel, 1=wavelength, 2=wavenumber,
                                    3=Raman shift)
show_mode;3                        //Y-axis option (0=Raw,1=Dark,2=Reference,3=Dark Subtracted,
                                    4=%TR, 5=Absorbance,6=Absolute Irradiance)
data_mode;0                         //Transmit data mode, 0=Binary, 1=ASCII (obsolete)
pixel_mode;0                       //Display Chart Mode .0=normal, 1=Pixel Monitoring (obsolete)
```

```
integration times(ms);1          //Spectrometer integration time of saved data
integration times unit;1         //Spectrometer integration time unit setting (0=us, 1=ms,
                                     2=sec, 3=min)
time_multiply;1                  //Spectrometer Integration time multiplier
average number;1                 //Number of spectral averages
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;0                  //Display Chart X-axis Minimum, if X-axis setting is Manual
xaxis_max;2047               //Display Chart X-axis Maximum, if X-axis setting is Manual
pixel_num;2048               //Sensor Pixel number
coefs_a0;372.651160422713        //The coefficients (A0) of Pixel convert to Wavelength
coefs_a1;0.273948279117576       //The coefficients (A1) of Pixel convert to Wavelength
coefs_a2;-3.32083876761757E-05   //The coefficients (A2) of Pixel convert to Wavelength
coefs_a3;-1.81673008524375E-09   //The coefficients (A3) of Pixel convert to Wavelength
coefs_b0;-2649.51440443471       //The coefficients (B0) of Wavelength convert to Pixel
coefs_b1;11.5617187502648        //The coefficients (B1) of Wavelength convert to Pixel
coefs_b2;-0.0166223418721358     //The coefficients (B2) of Wavelength convert to Pixel
coefs_b3;1.21997080526348E-05    //The coefficients (B3) of Wavelength convert to Pixel
coefs_r0;1                       //The coefficients (R0) of Pixel convert to Raman shift
coefs_r1;0                       //The coefficients (R1) of Pixel convert to Raman shift
coefs_r2;0                       //The coefficients (R2) of Pixel convert to Raman shift
coefs_r3;0                       //The coefficients (R3) of Pixel convert to Raman shift
coefs_j0;1                       //The coefficients (J0) of Raman shift convert to Pixel
coefs_j1;0                       //The coefficients (J1) of Raman shift convert to Pixel
coefs_j2;0                       //The coefficients (J2) of Raman shift convert to Pixel
coefs_j3;0                       //The coefficients (J3) of Raman shift convert to Pixel
enable_coefs_r;0                 //Use coefficient R0..R3 Enable. (0=Disable, 1=Enable)
laser_wavelength;0               //Raman excitation wavelength (nm)
laser_powerlevel;0               //Laser power level (percent)
probe_index;0                    //Probe index
probe_name;                      //Probe name
dark_compensate;0                //Dark compensate Enable.   (0=Disable, 1=Enable)
numcoeff_d;7                     //The order number of linearity correction
coefs_d0;0                       //The coefficients (D0) of linearity correction
coefs_d1;1                       //The coefficients (D1) of linearity correction
```

```
coefs_d2;0                      //The coefficients (D2) of linearity correction
coefs_d3;0                      //The coefficients (D3) of linearity correction
coefs_d4;0                      //The coefficients (D4) of linearity correction
coefs_d5;0                      //The coefficients (D5) of linearity correction
coefs_d6;0                      //The coefficients (D6) of linearity correction
coefs_d7;0                      //The coefficients (D7) of linearity correction
irradiance_lamp_inttime;1       //int time used when creating irradiance correction ratio
irradiance_lamp_unitindex;0     //lamp unit that used to crate irradiance correction ratio
Color_Data_Flag;0               //data source for calculation color (0=%TR, 1=absorbance)
Color_StartWL;400               //Start wavelength of calculation color
Color_EndWL;700                 //End wavelength of calculation color
Color_IncWL;10                  //Step wavelength of calculation color
power_unit_index;1              //Color 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)
Data Pretreat_0;                //Data pretreat process step 0
Data Pretreat_1;                //Data pretreat process step 1
Data Pretreat_2;                //Data pretreat process step 2
Data Pretreat_3;                //Data pretreat process step 3
Data Pretreat_4;                //Data pretreat process step 4
Data Pretreat_5;                //Data pretreat process step 5
Data Pretreat_6;                //Data pretreat process step 6
Data Pretreat_7;                //Data pretreat process step 7
Data Pretreat_8;                //Data pretreat process step 8
Data Pretreat_9;                //Data pretreat process step 9
Data Pretreat_10;               //Data pretreat process step 10
Data Pretreat_11;               //Data pretreat process step 11
Data Pretreat_12;               //Data pretreat process step 12
Data Pretreat_13;               //Data pretreat process step 13
Data Pretreat_14;               //Data pretreat process step 14
Data Pretreat_15;               //Data pretreat process step 15
```

```
Data Pretreat_16;                //Data pretreat process step 16
Data Pretreat_17;                //Data pretreat process step 17
Data Pretreat_18;                //Data pretreat process step 18
Data Pretreat_19;                //Data pretreat process step 19
Data Pretreat_20;                //Data pretreat process step 20
Data Pretreat_21;                //Data pretreat process step 21
Data Pretreat_22;                //Data pretreat process step 22
Data Pretreat_23;                //Data pretreat process step 23
Data Pretreat_24;                //Data pretreat process step 24
Data Pretreat_25;                //Data pretreat process step 25
Data Pretreat_26;                //Data pretreat process step 26
Data Pretreat_27;                //Data pretreat process step 27
Data Pretreat_28;                //Data pretreat process step 28
Data Pretreat_29;                //Data pretreat process step 29

Pixel;Wavelength;Wavenumber;Raman Shift;Dark;Reference;Raw data #1;Dark Subtracted #1;%TR
#1;Absorbance #1;Irradiance (lumen) #1;RelativeIntensityCorrection_Ratio #1;
ReferenceMaterialCorrection_Ratio #1;AbsoluteIrradianceCorrection_Ratio #1;
                                 //Header of data

0;372.65;26834.75;-
26834.75;1227.0000;65535.0000;1339.0000;112.0000;0.0000;0.0000;0.0000;1.0000;1.0000;1.0000;
               //pixel 0 data
```

Appendix B: Declaration of TXT File

The TXT 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 (highlighted by yellow). The flag block length may vary and an example of text file is shown below.

To read all data, the 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
baud1;3                             //baudrate index if spectrometer is RS232 interface
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, 1=ASCII (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
                                 (obsolete)
coefs_r1;-0.371893845826952      //The coefficients (R1) of Pixel convert to Raman shift
```

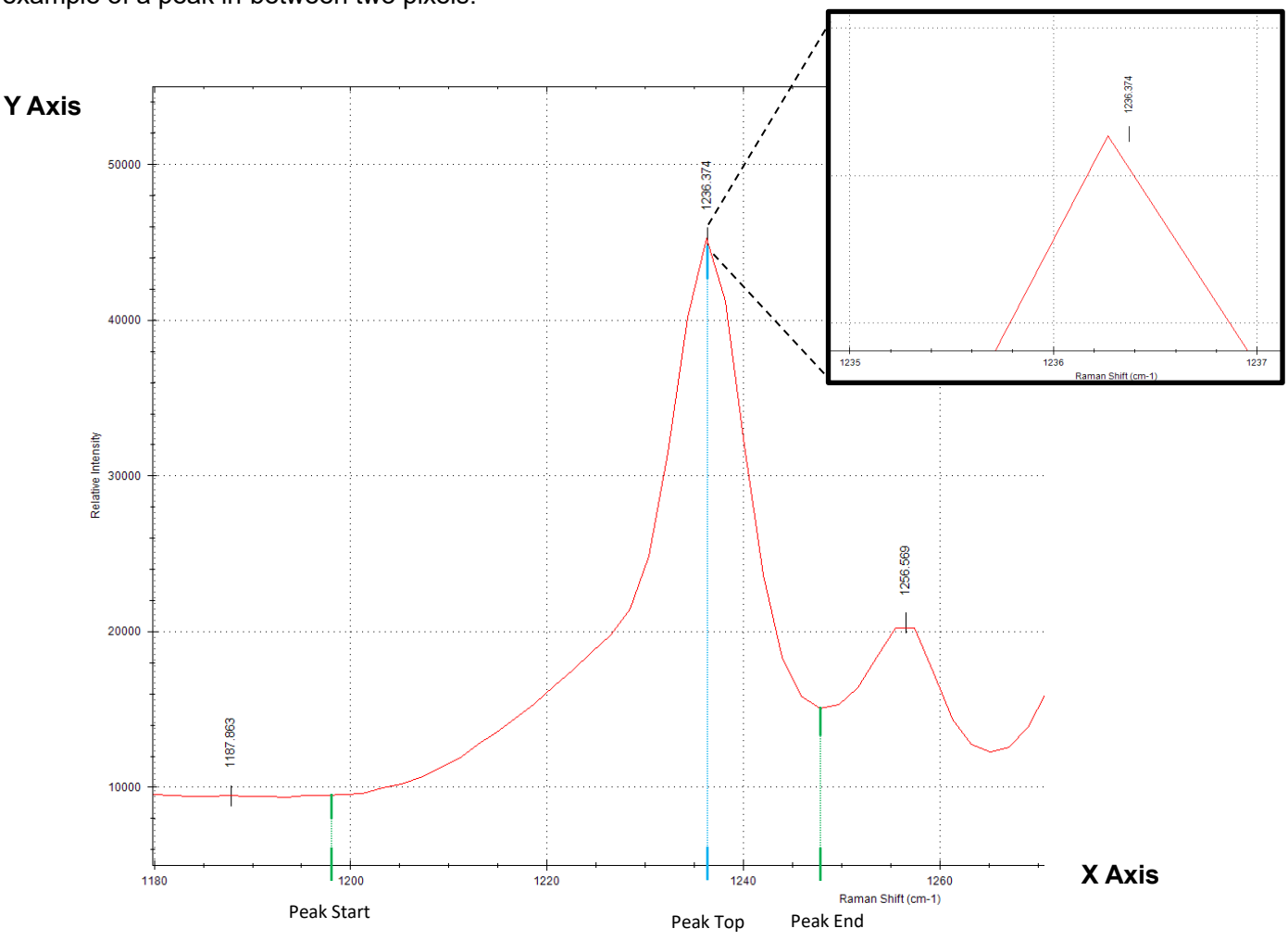
```
                                (obsolete)
coefs_r2;0.000853220967122155   //The coefficients (R2) of Pixel convert to Raman shift
                                (obsolete)
coefs_r3;3.37498265875635E-08   //The coefficients (R3) of Pixel convert to Raman shift
                                (obsolete)
coefs_j0;-112.640169933252      //The coefficients (J0) of Raman shift convert to Pixel
                                (obsolete)
coefs_j1;1.91244080985067       //The coefficients (J1) of Raman shift convert to Pixel
                                (obsolete)
coefs_j2;-0.000774766051834558  //The coefficients (J2) of Raman shift convert to Pixel
                                (obsolete)
coefs_j3;1.20204126521674E-07   //The coefficients (J3) of Raman shift convert to Pixel
                                (obsolete)
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;349.60        //(obsolete)
vertical_line4_wv;349.60        //(obsolete)
vertical_line_flag;0            //(obsolete)
vertical_line_ratio;0           //(obsolete)
```

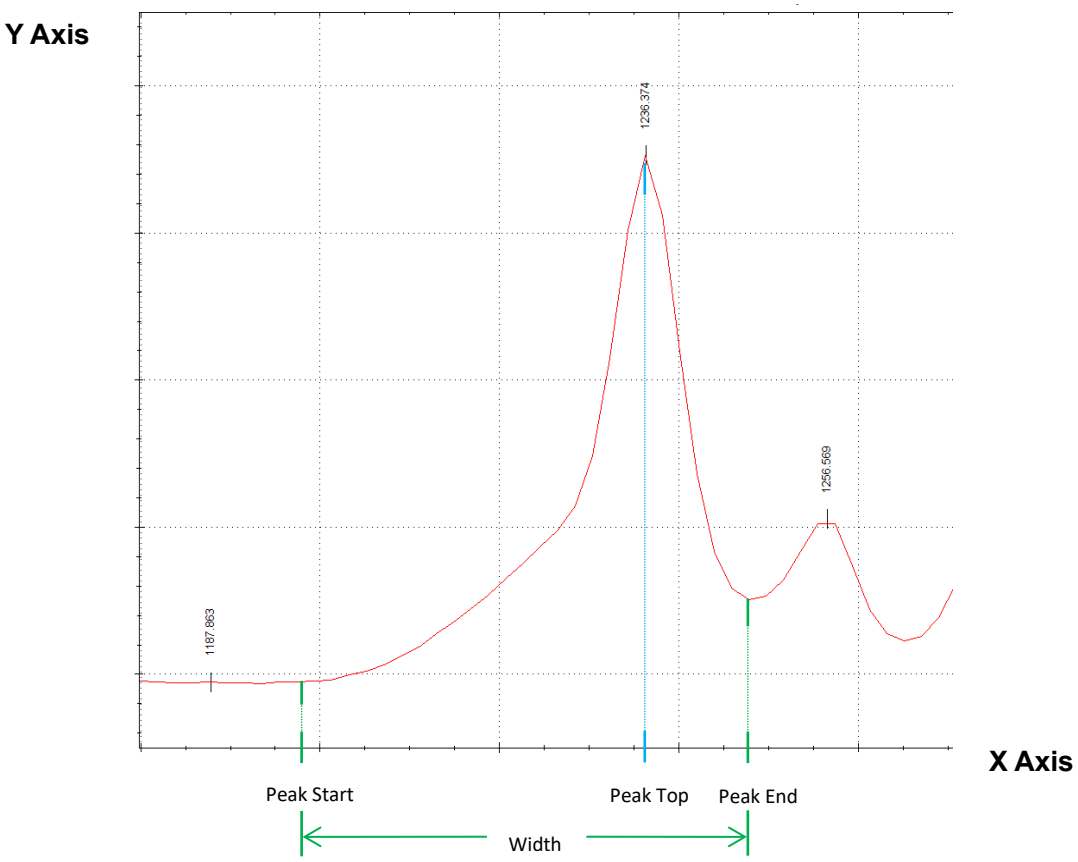
```
laser_wavelength;784.5            //Raman excitation wavelength, not used if enable_coefs_r=1
laser_powerlevel;0                //laser power setting
overlay_js;0                          //(obsolete)
Relative Intensity Correction Flag;0  //(obsolete/not defined)

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;etc.
```

Appendix C: Peak Property Values

This is an overview of Peak Position and Properties, used in Peak Analysis and Peak Monitor Setup (Basic Measurement Type). Peak position is determined by curve fitting, instead of using the position of the highest pixel. This allows for a more accurate representation of the actual peak, and becomes more obvious when a peak lands in-between adjacent pixels - with one pixel usually being slightly higher than the other – and the peak calculated accordingly.
In Peak Analysis, the peak is determined by the Minimum Absolute Height and Minimum Peak Width criteria.
In *Peak Monitor Setup, the highest point found within the Start and End Position will be taken as the peak.*

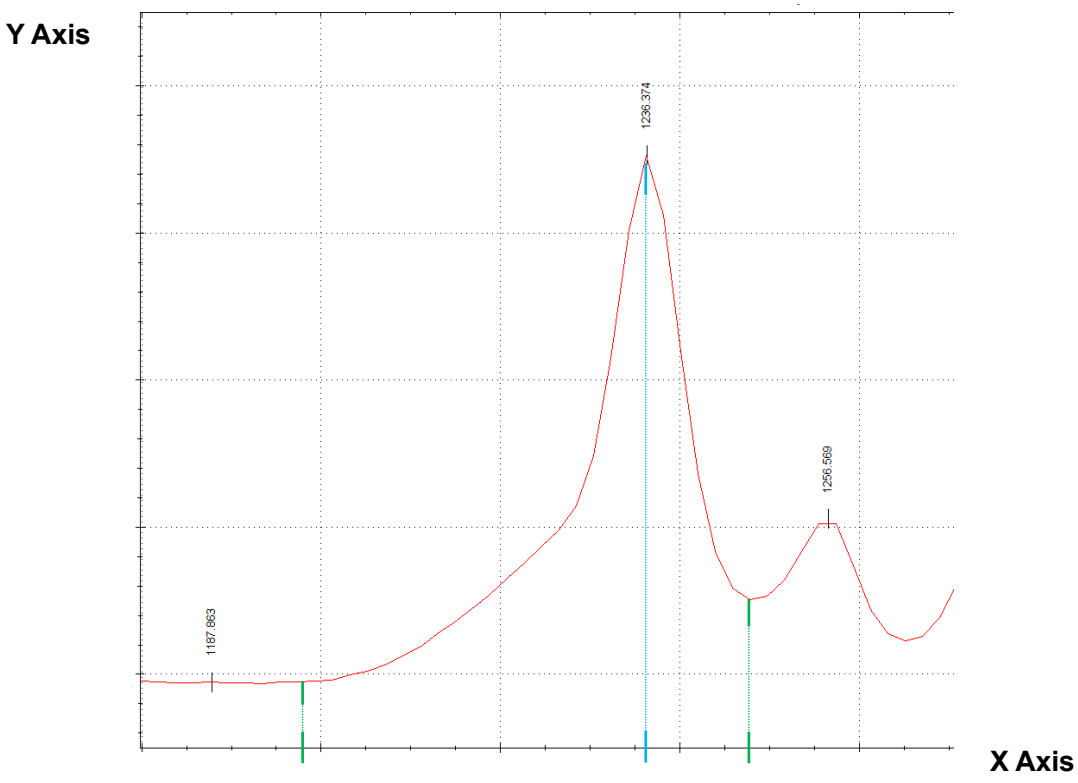
The following examples use a practical example of the 1236 cm^{-1} peak of a standard Acetaminophen (Tylenol) sample. The curve fitted peak position is 1236.374 cm^{-1}, while the highest pixel is 1236.3 cm^{-1}, refer to the close up of the peak. This peak was chosen because of its closeness to its neighboring 1257 cm^{-1} peak, giving an uneven looking peak to better visualize the peak picking algorithms. The 1257 cm^{-1} peak also gives a perfect example of a peak in-between two pixels.



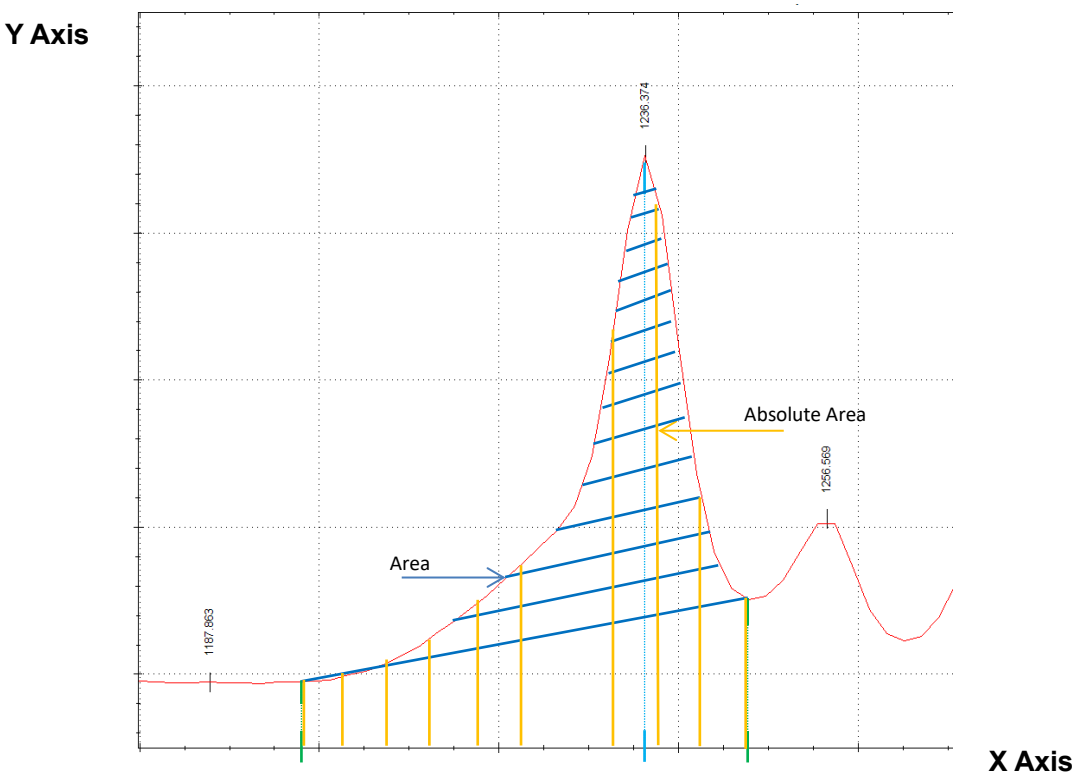


Peak Monitor Setup's Basic Measurement Type provides options for determining where on the peak to measure and what units are being measured. The **Start** and **End** of a peak is determined by the beginning rise of the peak compared to the baseline (left side), or the sudden rise of the next peak (right side). The **Top** of the peak is determined by curve fitting. Here is a simplified breakdown of the options; for example the **Ramanshift Start** gives the x-axis Raman Shift value of the beginning of the peak, and is found to be 1197 cm^{-1}.

Peak Start: The x-axis value of the beginning of the peak (left side).
Peak Top: The x-axis value of the curve fitted peak position.
Peak End: The x-axis value of the end of the peak (right side).
Width: Subtraction of Peak Start from Peak End.
Peak (Ramanshift): Gives the Raman Shift value (X Axis)
Peak (Wavelength): Gives the Wavelength value (X Axis)
Peak (Wavenumber): Gives the Wavenumber value (X Axis)
Peak (Pixel): Gives the Pixel value (X Axis)



Peak FWHM: Full Width of the peak's Half Maximum. Calculated beginning from half the peak's height on each side, then the width of those half height values.
Height: Y-axis value of Peak Top measured from the calculated baseline.
Absolute Height: Y-axis value of Peak Top measured from zero.
Height %: Peak height divided by the sum of all peaks height
Absolute Height %: Absolute height divided by the sum of all peaks absolute height.



Area: Area is defined by the Height (above baseline) and Width; blue shaded area.
Absolute Area: Area is defined by the Absolute Height and Width; yellow shaded area.
Area %: Area divided by the sum of all peaks Areas.
Absolute Area %: Absolute Area divided by the sum of all peaks Absolute Areas.
Fitted Curve X: Performs a fitted curve splining between the 2 set points and reports the center X value.
Fitted Curve Y: Performs a fitted curve splining between the 2 set points and reports the center Y value.
Manual Peak Area: Manually select the baseline removal points and calculated area start end end.

Appendix D: 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 E: Irradiance Ratio File Data Definition

Ratio1_ccode.txt File details and explanation of data:

RATIO1_ccode.TXT INFORMATION	EXPLANATION
BWSpec Version=BWSpec 4.04	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	