

BWSpec[®] 4.11 Software User Manual

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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.

There are significant changes from previous versions. Existing users using **BWSpec v4.04 or lower** should pay attention to the following notable differences in **BWSpec v4.10+**:

- New application-based Workspace introduced. The software now has 2 workspaces selectable by the user: BWSpec and Raman. The BWSpec workspace retains the original look. Changes in Raman workspace include:
 - a. Irrelevant x-axis unit types are removed from Spectrometer Control Panel, including Wavelength (nm), Wavelength linear(nm), Wavenumber linear(cm-1).
 - b. Irrelevant y-axis types are removed from Spectrometer Control Panel, including Reference, Transmission/Reflectance, Absorbance, and Absolute Irradiance.
 - c. Unused outputs are removed Acquire Controls: output 2, 3, 4, and 5.
 - d. Irrelevant utilities are removed from the tools menu, such as Linearity Correction, Irradiance Calibration, Reference Material Correction, and System Response Standardization.
 - e. Dark Compensate option is removed from the Acquire menu.
 - f. Acquire Reference is removed from the tool bar.
 - g. Dark spectrum is required to complete an acquisition, and it must have the same integration time as the signal spectrum to ensure proper subtraction.
- Added drag and drop function for opening spectral files. Such files can be opened by selecting from Windows Explorer and dropping into the Graph window.
- Added a new file type TXTR, which has an extra data block to store the Relative Intensity Correction ratio spectrum. This ensures the integrity of spectral files and makes it easy to transport and reprocess them without loss of critical information.
- Added data processing audit trails to TXTR spectral file header to record the treatment steps for the Processed Data block starting from the Raw Data block. These are the numbered Pretreat lines and can be viewed in Spectrum List Panel.
- Added Probe Setup tab to Hardware Setup under Setup menu to configure probes.
- Added Experiment Setup in Setup to save data acquisition and treatment configurations. These configuration files can be loaded to reproduce previous experiment conditions.
 - a. Added Probe selection to Experiment Setup to allow easy selection of probes from a list of probes pre-configured in Setup/ Hardware Setup/ Probe Setup.
 - b. Added Spectral Processing function to Experiment Setup to perform predefined data processing.
 - c. Added Analytics function to Experiment Setup to perform predefined data analysis.

- d. Improved Timeline function and added it to Experiment Setup to perform kinetic measurements and analysis.
- Added safeguard to prevent Raw Data and Dark data blocks from being altered by data processing. Only Processed data block can be altered by data processing.
- Replace linear interpolation with cubic spline interpolation for improved fidelity.
- Improved peak analysis precision. Peak position is accurately determined by curve fitting, instead of using the position of the highest pixel.
- In Spectrum List Panel, removed the distinction of “Measured Spectra” and “Open Spectra”. Removed file management tools “Rename Selected spectrum”, “Save Selected Spectrum”, and .
- Established rules for spectral file management in Spectrum List Panel.
 - a. A new spectral file cannot be created until all necessary elements for the last acquired spectrum are complete. For example, in Raman Workspace, a dark spectrum must be present and must be acquired with the same integration time as the signal spectrum.
 - b. A Saved or Finished spectrum can no longer be overwritten by acquiring new data.
- Reorganized Tools Menu and added a new Spectral Function menu. Old Tools menu included both Instrument Utility Tools such as creating calibration references, and spectral processing functions, some of which are automatically applied to new acquisitions in an undefined manner. The new tools menu only includes Instrument Utility Tools. The new Spectral Function menu provides data processing functions that are applied only to selected spectra, not to new acquisitions. The Spectral Function can only be applied to the Processed Data block, and are disabled unless the active Y Axis Type is set to Processed Data. Data processing functions to be applied to new acquisitions are defined in Experiment Setup/ Spectral Processing/ Additional Processing.
- Removed Option menu, which included both Instrument Utility Tools (such as creating calibration references) and spectral processing settings (such as enable/disable various calibrations). Instrument Utility Tools are moved to Tools menu, and spectral processing settings set moved to setups: Experiment Setup for new acquisitions, and Batch Re-Process for saved spectra.
- Added Batch Re-Process function to Spectral Function menu to allow re-processing the data starting from the raw data.
- Timeline Load function Improvement: added Batch Re-Process to allow reprocessing and re-analyzing the data.
- Improved Peak Analysis.
 - a. Peak position is accurately determined by curve fitting, instead of using the position of the highest pixel.
 - b. Removed data source selection. Only the active Y-axis Type of the Selected Spectrum is labeled and reported.
 - c. Added Report Export and Printing function.
 - d. Standardized the parameter name and corrected inconsistencies.
 - e. When Baseline Removal is checked, analysis results is now based on the baseline subtracted

spectrum.

- Hardware Setup
 - a. Removed the option “Close LED Illumination on Data Scan”. LED Illumination is always automatically turned off during spectral acquisition including dark scan.
 - b. Replaced the option “Open Laser Before Data Scan, Close Laser After Data Scan” with “Open Laser Before Data Scan”.
 - c. Added Laser Timeout in Common Setting to extend laser lifetime. If the laser has been idle in the On state for a period equal to the timeout period, laser will be automatically turned off.
 - d. Added a tab “Probe Setup” to pre-configure probes for the system. Relative Intensity Correction ratio file for Raman application must be configured here for it to be saved in the TXTR file format and applied following data acquisition. Although not mandatory for data acquisition, this is strongly recommended for Raman application.
- Spectral Function/Baseline Removal: changed the Lambda scale bar from linear to logarithmic for improved sensitivity.
- Added integration time units.
- Renamed Irradiance Correction to Irradiance Calibration.
- Removed Dark Compensate from Acquire menu in Raman Workspace.

Notable Bug Fixes

- Baseline Removal: fixed the bug that the result spectrum and the preview did not agree with each other.
- Sawitzky-Golay derivative: fixed the bug that window size (points) had no effect on the results, and even integers were accepted.
- Firmware revision for BTC261P and BTC264P fixed the acquisition and readout delay at shorter integration times.
- In previous versions, when auto time and external trigger are both selected, the trigger only works when it's pressed a second time. This is now fixed.
- i-Raman Pro: modified the warmup behavior. Data can now be acquired during instrument warmup.
- Improved External Trigger Pacing Mode behavior. In some spectrometer models (BTC665N, BTC667N), this mode does not work with very short integration times, because these models are Level Triggered, while the manual trigger typically cannot be released before the current acquisition is finished, causing multiple acquisitions to be done for a single triggering event. Now, a 0.5 second delay is added between acquisitions to give the user enough time to release the trigger.

Known Bugs

- Timeline chart time axis is relative to the time of first spectrum acquisition, not in real time.

- Spectrum cannot be saved with a file name already in use by another one listed in Spectrum List Panel.
- In Spectrum List Panel if a spectrum name is expanded to show the details and it is at the top of the field, clicking the "-" to collapse the field can uncheck all spectra.
- Peak Analysis: peak analysis cannot be performed for TXTR and TXT files when X Axis unit is Wavelength Linear, Wavenumber Linear, or Raman Shift Linear.
- If you have open ANY file of file name "example1", then you take a new spectra, and try to save this spectra with the name "example1" in a DIFFERENT FOLDER LOCATION, you get an error "This Spectra name already be used". This error does NOT appear if trying to open 2 files with the same name from DIFFERENT folder locations.
- The Spectrum List Panel treats an "Unclick" as a click. This means, when you go to expand the details of a spectra, go to click the "+" again, the checkbox for All spectra under the Spectrum List will get unchecked as you "Unclick"
- Calculation for v' is incorrect. This can be tested with the Irradiance Setup
- BTC261P Pixel Mode setup against i-Spec (BWS903). There was a bug which caused only half the spectrum to be read instead of every other pixel.
- 3d Graph Feature; update the dll to be supported by Windows 8/8.1

In addition to the above, **BWSpec v4.11** includes the following changes and fixes:

- Added Manual Peak Area Calculation in Experiment => Peak Monitor Setup
- Additional Scan Run information now can be saved in *.txtr files. Enable this option for each scan under Experiment setup.

Notable Bug Fixes in **BWSpec v4.11**:

- The issue with some computers in setting the TE Cooler temperature for some spectrometers when the computer is setup with the European Number Format has been fixed.
- Pulse Output now properly calculates the total pulse train against the set integration time.
- File conversion from *.txt to *.txtr is now more stable.
- Switching to Japanese language now supports more spectrometer models.
- Loading Experiment Setup is now more reliable with different configurations.

Known Bugs in **BWSpec v4.11**:

- Enabling BAC151x plug-ins will cause spectrometers with built-in shutters to automatically close the shutter during normal scan. Disable the BAC151x plug-in in order to use these spectrometers.

2 INSTALLATION

3 SUPPORTED OPERATING SYSTEMS

Windows 7 (32 bit & 64 bit)

Windows 8 / 8.1 (32 bit & 64 bit)

Windows 10 (32 bit & 64 bit)

4 MINIMUM SYSTEM REQUIREMENTS*

Meets or exceeds the System Requirements for your PC's Operating System respectively

Processor: 1.5GHz or faster

RAM: 1GB or more

Hard disk space: 250MB available or more**

* The requirements are for normal use and do not include resource intensive features like Burst Mode

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

5 SOFTWARE & HARDWARE INSTALLATION

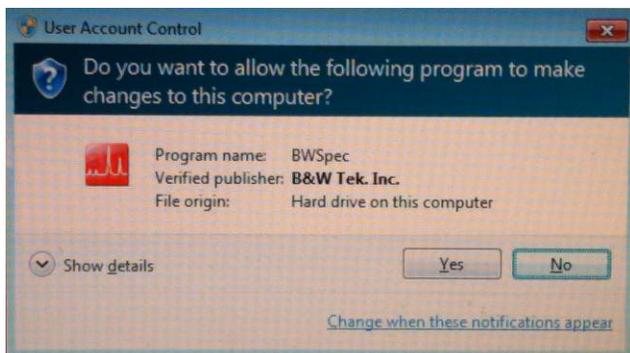
- Refer to “BWSpec Software and Hardware Installation Guide” for fully detailed installation instructions:
- Insert the BWSpec 4 USB Flash Drive into the computer's USB port and copy the installation file to local computer.
- Install the software;
- After software installation, **DO NOT** open the BWSpec program;
- Connect the spectrometer to the PC via an USB Cable;
- Install the Hardware Driver(s) for the spectrometer;
- After hardware driver installation, open/run the BWSpec program.
- To get started with a Raman System, go to Section 15.7 Experiment Setup for a walk-through example.

6 RUN BWSPEC

Double click the BWSpec icon on the desktop:

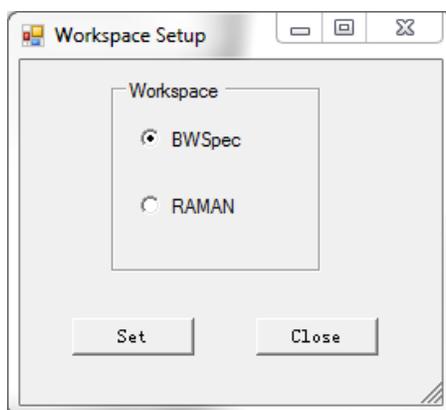


If the User Account Control is active, the following message will appear:



Click **Yes** to continue.

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



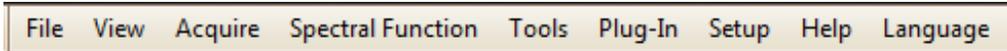
If you are unsure, choose the default **BWSpec** workspace and click **Set**. This option may be changed later within the main program; Setup → Workspace.

7 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.

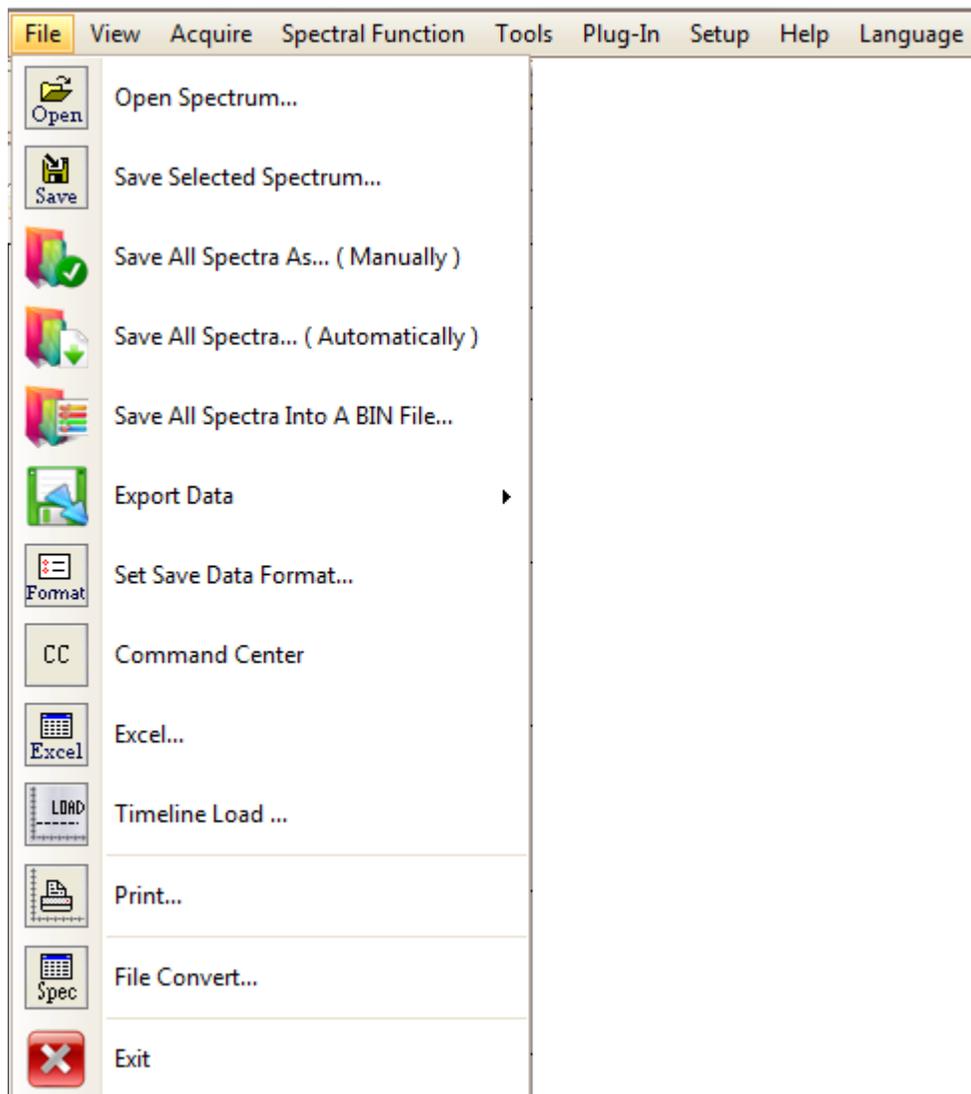
The screenshot displays the BWSpec 4 software interface. At the top is the **Menu Bar** (Sec. 8) with options: File, View, Acquire, Spectral Function, Tools, Plug-In, Setup, Help, Language. Below it is the **Toolbar** (Sec. 18) containing icons for Open, Save, Excel, and various acquisition controls. The main window title is "Sys Model.BRC115P Color Chart Sec. 25". The central plot shows a red spectral curve with "Relative Intensity" on the y-axis (0 to 60,000) and "Wavelength (nm)" on the x-axis (200 to 800). The plot title is "C-code : File Name : Data Type → ZLNA : SP_1 : Raw Data". To the right is the **Spectrum List Panel** (Sec. 19) showing a list with "RSP_1" selected. Below that is the **Spectrometer Control Panel** (Sec. 21) with options for "Enable Cursor", "Dual Chart", and "Display Options" (X Axis Unit: Wavelength (nm), Y Axis Type: Raw Data). At the bottom is the **Status Bar** (Sec. 22) showing "Online", "59", "Acquisition stopped", and various status indicators. A **Spectrometer Information Panel** (Sec. 20) is partially visible at the bottom right, showing "Pixel = 1590, Wavelength (nm) = 769.38, Wavenumber (cm-1) = 12997.48, Raman Shift (cm-1) = -258.6, Relative Intensity = 1445".

8 MENU BAR



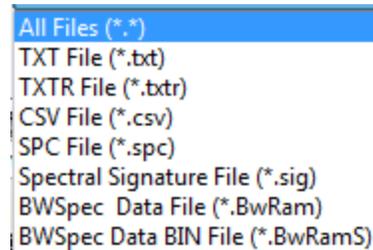
The following sections are detailed descriptions of the dropdown menus available for each menu option in the BWSpec 4 Menu Bar.

9 FILE



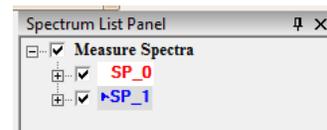
9.1 Open Spectrum...

-  Open Spectrum...
- Load a previously saved spectral file into the main graph.
- Available in the following formats:
 - TXT File (*.txt)
 - TXTR File (*.txtr)
 - CSV File (*.csv)
 - SPC File (*.spc)
 - Spectral Signature File (*.sig)
 - BWSpec Data File (*.BwRam)
 - BWSpec Data BIN File (*.BwRamS)
- Data from other instruments and software saved in SPC format can also be opened in the BWSpec software.



9.2 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:
 - *.txt
 - *.txtr
 - *.csv
 - *.txt(Even)
 - *.spc
 - *.BwRam



9.3 Save All Spectra As...(Manually)

-  Save All Spectra As... (Manually)
- Save all the spectra listed in the **Spectrum List Panel** individually
- A new Save Spectrum Data window will open for each spectrum.

9.4 **Save All Spectra...(Automatically)**

-  Save All Spectra... (Automatically)
- Save all the spectra in the **Spectrum List Panel** at once.
- The save name is the name used in the **Spectrum List Panel**.

9.5 **Save All Spectra into a BIN File...**

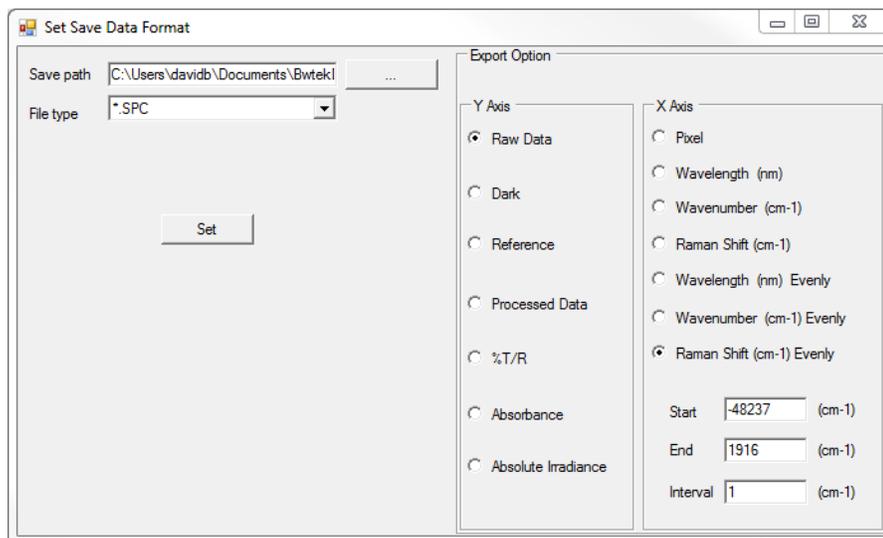
-  Save All Spectra Into A BIN File...
- Save all the spectra in the **Spectrum List Panel** into one BIN file with *.BwRamS file extension.

9.6 **Export Data**

-  Export Data
- Export all spectral data into one text file.
- Set the type of data and format.
- This function needs to be enabled through **Plug-In Manager**.
- Refer to Section 24.3 for more details.

9.7 Set Save Data Format...

-  Set Save Data Format...
- Configures the default **File type** when saving spectra.
- Sets the default **Export Option** for file types ***.txt (Even)** and ***.spc**
- Other file types automatically save all data, as seen in the “**Save Spectrum**” checklist tree.



9.8 Command Center

-  Command Center
- For importing spectral signatures for analysis and exporting Library updates.
- This feature is only for use with the handheld Raman series TacticID.
- Refer to the TacticID User Manuals for more information.

9.9 Excel

-  Excel...
- Export the active/selected single spectrum from the **Spectrum List Panel** to an Excel sheet.
- The file will open in Excel when the export is complete.
- Supported in all Excel versions.

9.10 **Timeline Load ...**

-  Timeline Load ...
- Automatically loads the files that were saved previously in **Timeline**.
- May be used with **Batch Process** to reprocess the data as you load it into BWSpec.
- **Load path** selects the folder location for the timeline data set.
- The corresponding files are displayed on the **Spectrum List Panel**.
- Refer to Section 24.12 for more details on Timeline

9.11 **Print...**

-  Print...
- Opens **Print Preview** window with the displayed data and header information.
- The user can make changes and add a watermark.
- Options to print, export document, or send as an e-mail.

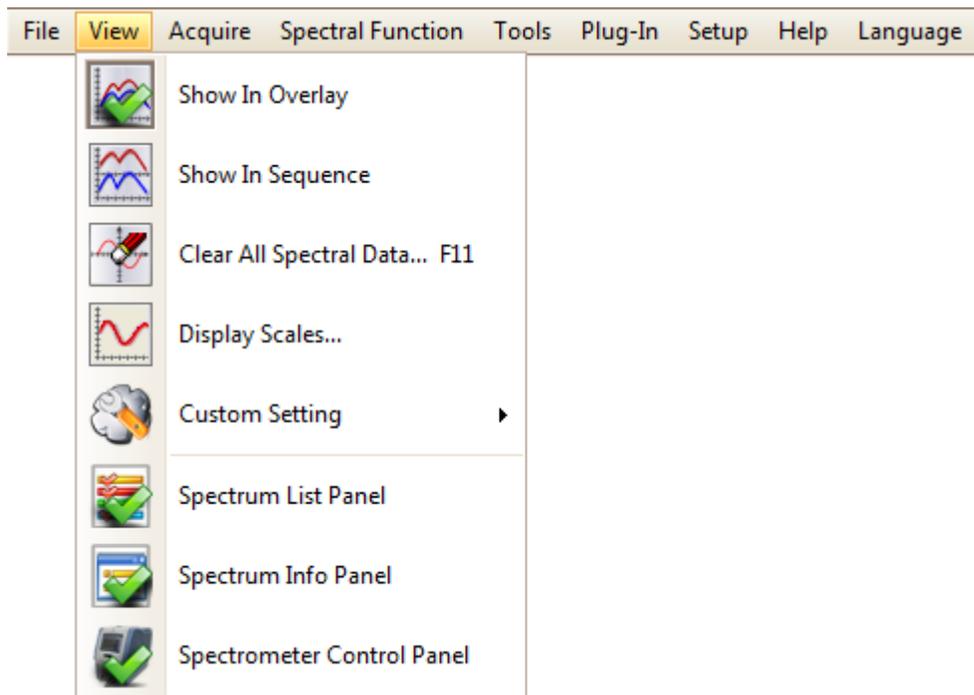
9.12 **File Convert...**

-  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.
- Must use the appropriate Ratio files for the conversion to have the corrections applied.
- Any processing done in the *.txt file will not be recorded in **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.

9.13 **Exit**

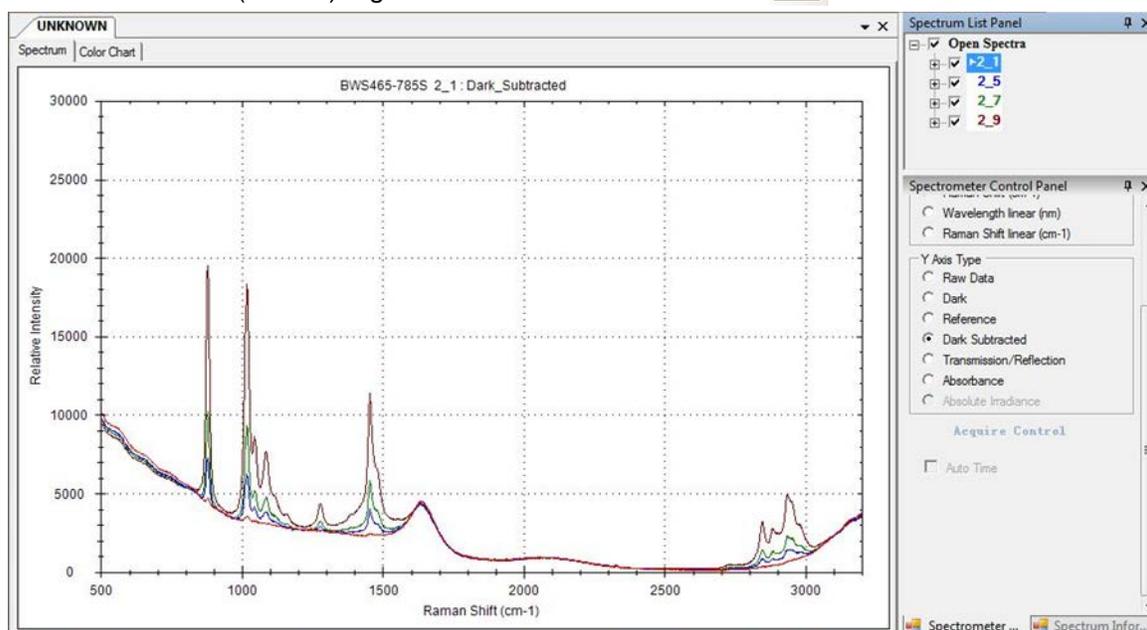
-  Exit
- Closes the BWSpec program.
- You will be prompted to save any unsaved or modified spectra.

10VIEW



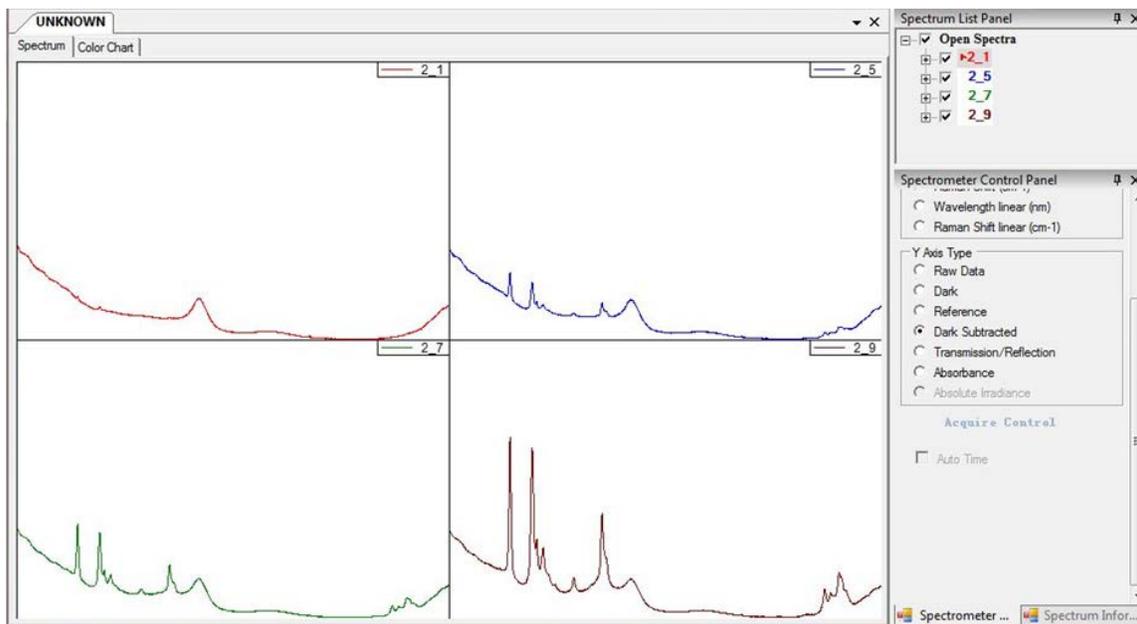
10.1 Show In Overlay

-  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 Overlay



10.2 Show In Sequence

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

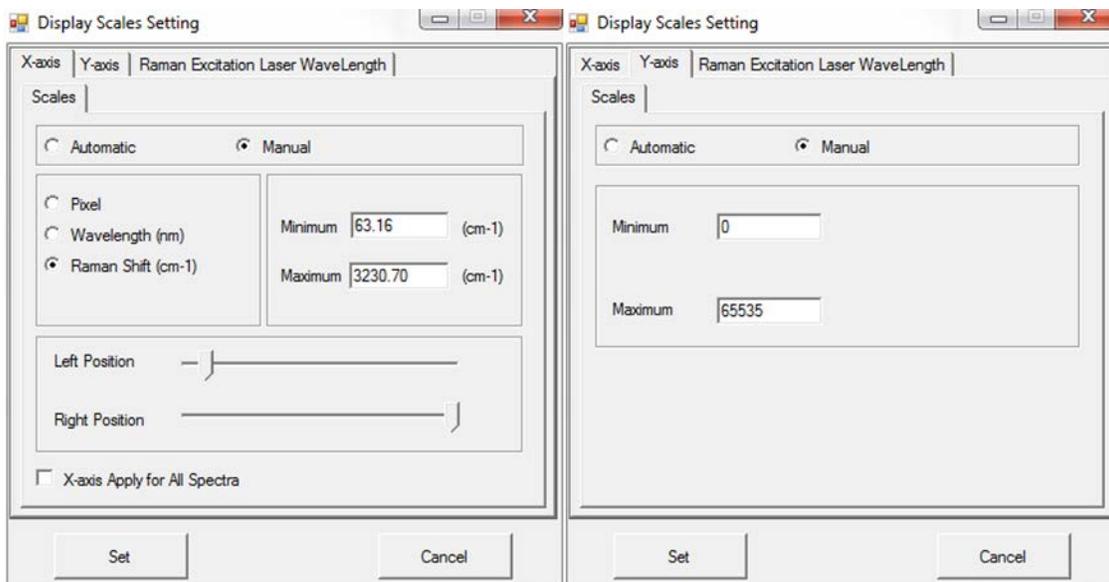


10.3 Clear All Spectral Data...

-  Clear All Spectral Data... F11
- Remove all spectra from the **Spectrum List Panel**.

10.4 Display Scales...

-  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.
- The Raman Excitation Laser Wavelength is for Raman only. **Do not adjust this value. This will change the Raman Shift calculation.**

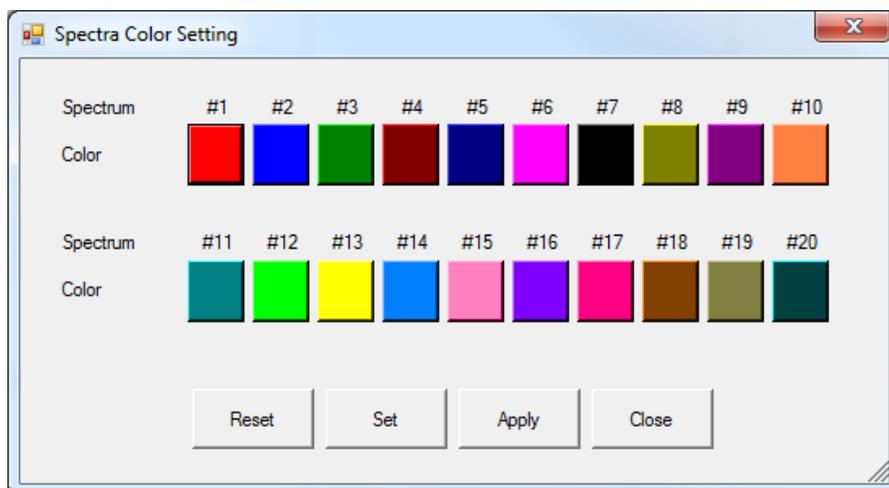


10.5 Custom Setting

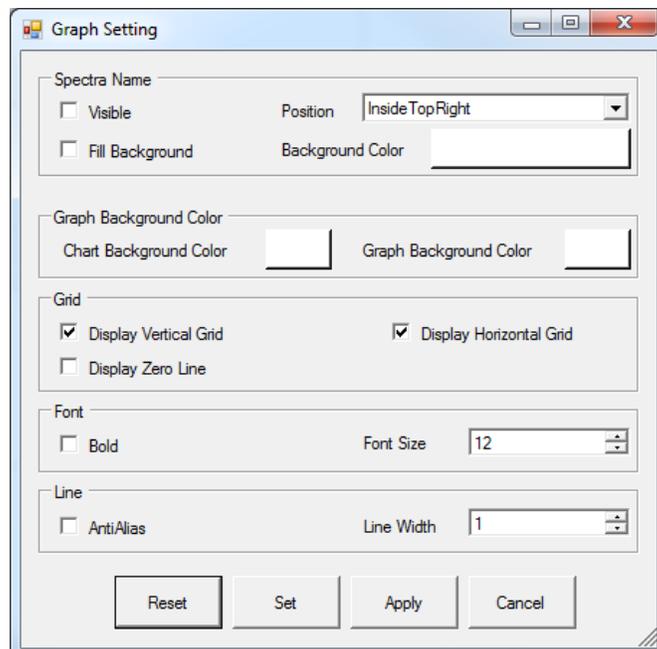
- 
 -  Spectra Color Setting...
 -  Spectra Graph Setting...

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.

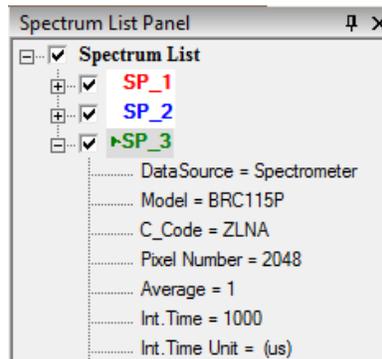


- Spectra Graph Setting...**
 - Opens a **Graph Setting** window where the variables relating to the graph window display can be set and adjusted to create a customized graph.



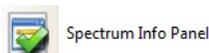
10.6 Spectrum List Panel

-  Spectrum List Panel
- Toggles On/Off display of the **Spectrum List Panel** on the right side of the display.
- Spectrum with the arrow  next to the name is the “active” spectrum and the current data is overwritten if additional spectra are taken.
- After an Overlay spectrum is taken, the previous spectrum cannot be modified. For example, after SP_3 is taken, SP_1 and SP_2 cannot be modified.
- 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 Section 19 for more details.

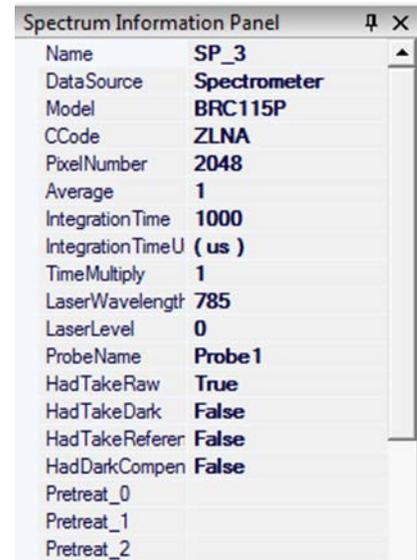


10.7 Spectrum Information Panel

-  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.



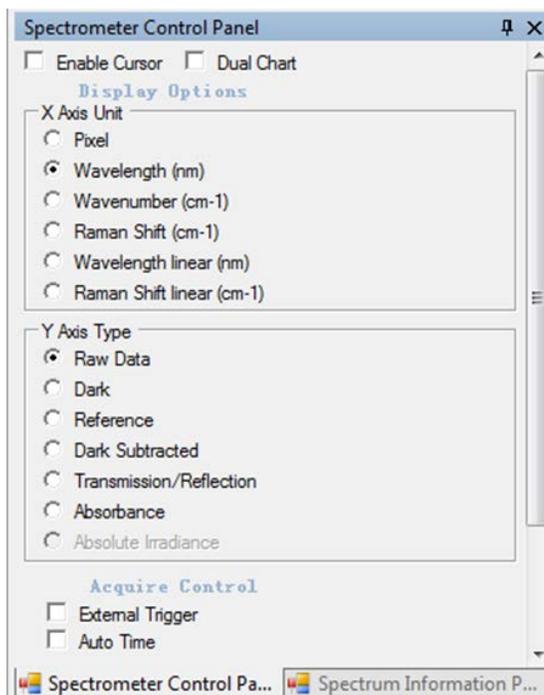
- Refer to Section 20 for more details.



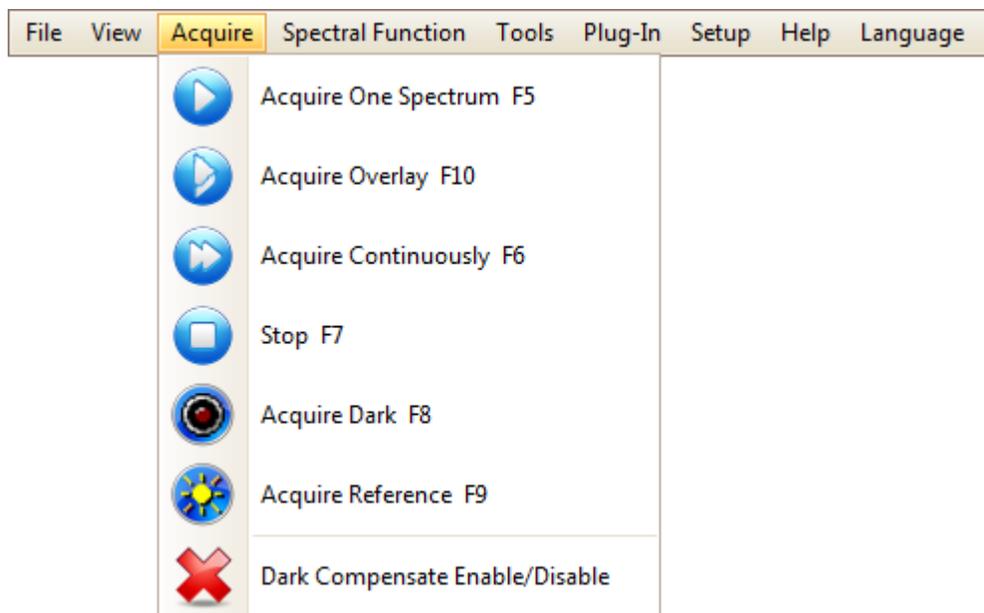
Spectrum Information Panel	
Name	SP_3
DataSource	Spectrometer
Model	BRC115P
CCode	ZLNA
PixelNumber	2048
Average	1
Integration Time	1000
IntegrationTimeU (us)	
TimeMultiply	1
LaserWavelength	785
LaserLevel	0
ProbeName	Probe 1
HadTakeRaw	True
HadTakeDark	False
HadTakeReferer	False
HadDarkCompen	False
Pretreat_0	
Pretreat_1	
Pretreat_2	

10.8 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.  Spectrometer Control Panel
- Refer to Section 21 for more details.



11 ACQUIRE



11.1 *Acquire One Spectrum*

-  Acquire One Spectrum F5
- Acquires a single spectrum from the spectrometer and displays it on the graph.
- The data is viewable on the **Raw Data Y Axis Type**.

11.2 *Acquire Overlay*

-  Acquire Overlay F10
- 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**.

11.3 *Acquire Continuously*

-  Acquire Continuously F6
- 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**.

11.4 Stop

-  Stop F7
- Stops acquisition while using **Acquire Continuously**.

11.5 Acquire Dark

-  Acquire Dark F8
- Acquires a single spectrum which is stored as the **Dark** array.
- The Dark array is viewable in the **Dark Y Axis Type**.

11.6 Acquire Reference

-  Acquire Reference F9
- Acquires a single spectrum which is stored as the **Reference** array.
- The Reference array is viewable in the **Reference Y Axis Type**.

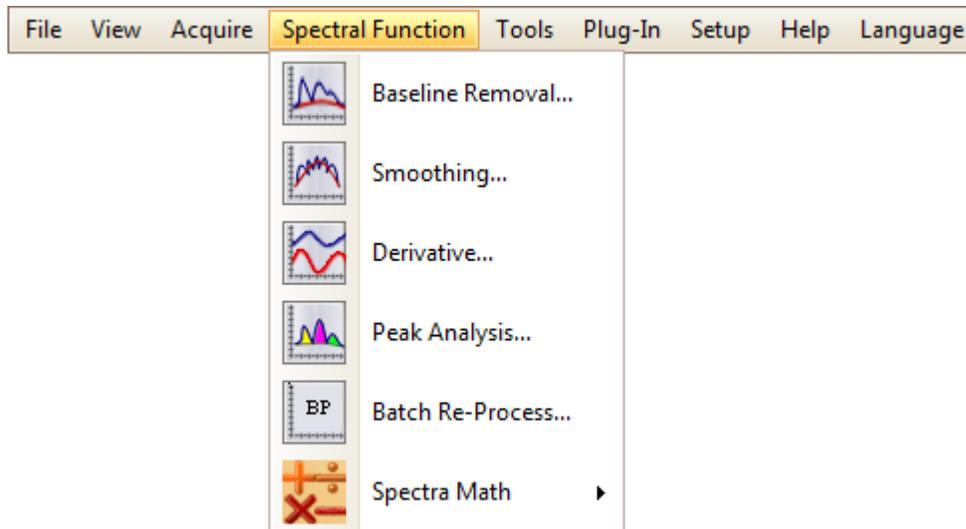
11.7 Dark Compensate Enable/Disable

-  Dark Compensate Enable/Disable
- The **Dark Compensate** feature provides an electronic dark reference array that is available with select spectrometers.
- This is a close approximation to the average level of a true dark spectrum, but does not contain the pixel to pixel variations,
- When applied, the **Dark** array is subtracted from acquired spectra (**Raw Data**).
- The applied **Dark Compensate** is viewable in the **Dark Subtracted (Processed) Y Axis Type**.
- This function is ideal for conditions where dark subtract is inconvenient to use (long integration times or during constant exposure conditions).
- **Dark Subtract** and **Dark Compensate** are mutually exclusive. If a **Dark** array is used, **Dark Compensate** will not be applied.
- **Dark Compensate** is not available in **Raman Workspace**.
- When enabled, a green checkmark is shown.  Dark Compensate Enable/Disable

11.8 **Acquisition Tips**

- The “active” spectrum will have the current data overwritten if additional spectra are taken.
- A **Dark Spectrum** is used to subtract the contribution (dark noise) of the sensor itself. This is carried over until a new dark spectrum is acquired.
- A measured spectrum is unfinished when it is just acquired. It becomes Finished after it is saved to a disc, 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, such as, 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.

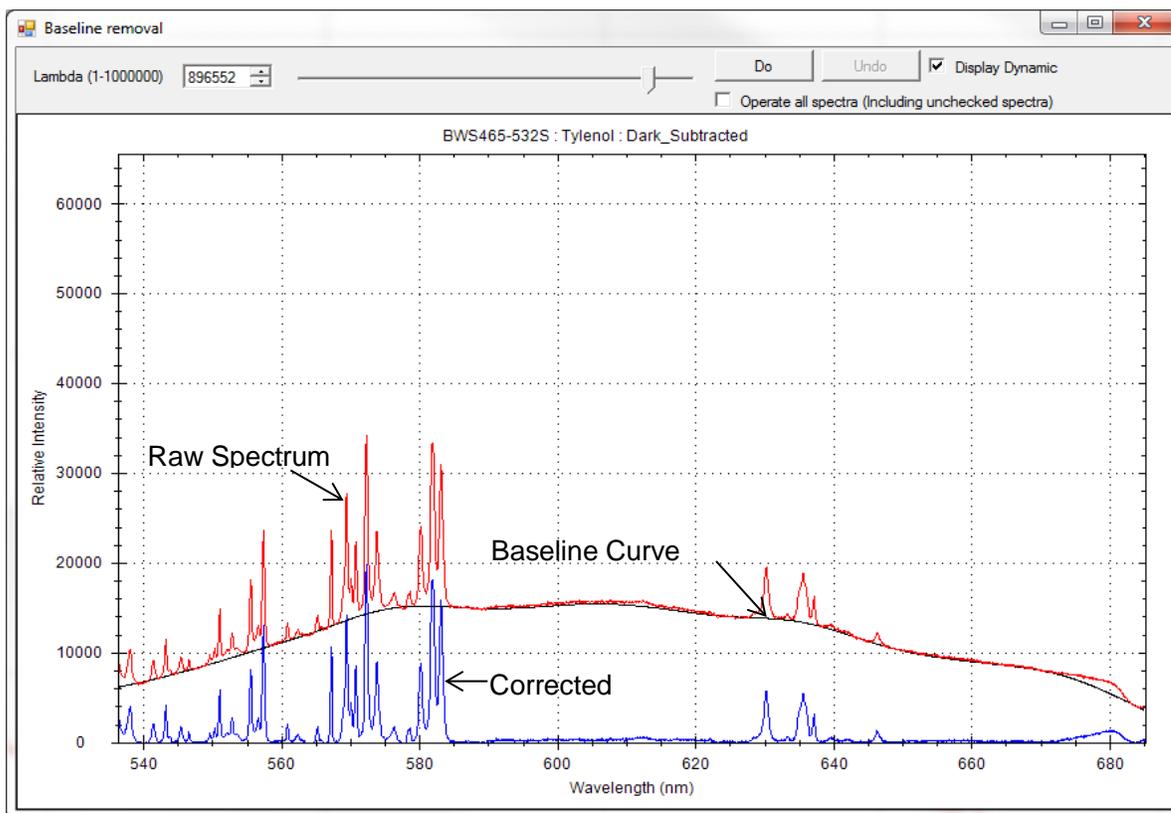
12 SPECTRAL FUNCTION



- The default items in the **Spectral Function** menu are **Smoothing**, **Derivative**, **Peak Analysis**, and **Batch Re-Process**. **Background Removal** and **Spectra Math** will become visible in the menu after being enabled in the **Plug-In Manager**.
- These functions work on all spectra Checked in the **Spectrum List Panel**.
- 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. **Peak Analysis** does not alter the data and is enabled on these **Y Axis Types**.

12.1 Baseline Removal...

-  Baseline Removal...
- The **Baseline Removal** function is used to perform baseline correction.
- This function is disabled when the **Y Axis Type** is set to **Raw Data**, **Dark**, or **Reference**.
- A preview window with three spectra will be displayed: raw spectrum (red), automatically fitted baseline curve (black), and the spectrum after background removal (blue). The color of the raw spectrum 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.
- Enable this function in the **Plug-In Manager**.

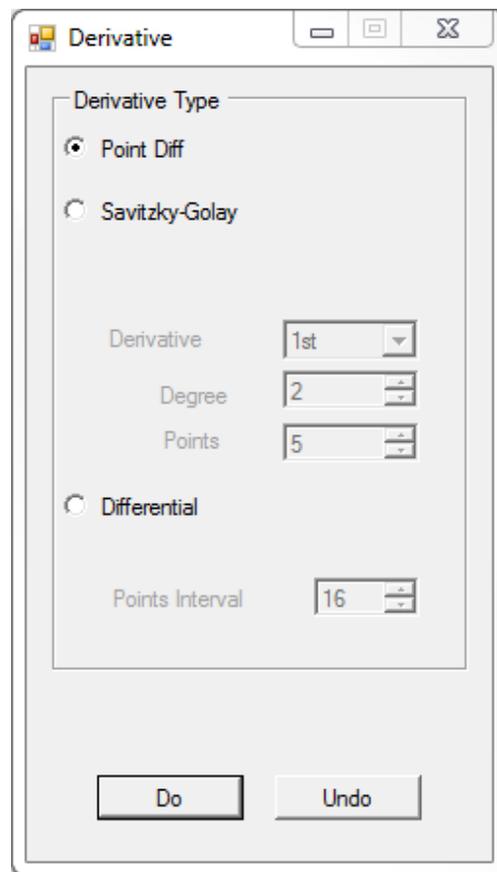


12.2 Smoothing...

-  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**.
- **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 in order to preserve the needed spectral information.

12.3 Derivative...

-  Derivative...
- Opens a **Derivative** window for applying derivatives to all displayed spectra.
- This function is disabled when the **Y Axis Type** is set to **Raw Data**, **Dark**, or **Reference**.
- **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.



12.4 Peak Analysis...

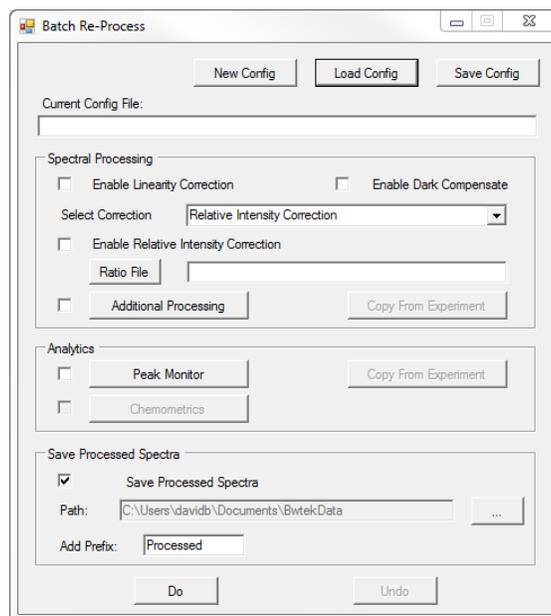
-  Peak Analysis...
- Information on peaks in the spectrum can be shown live in the software's display window.
- **Automatic Peak Identification**; Peak position is accurately determined by curve fitting, instead of using the position of the highest pixel.
- In the top left-hand corner of the menu, input 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 or modify a peak manually**. Then go to the main graph and click and drag a box over the peak of interest.
- Select the **Report Export** button  to export table to an Excel sheet.
- Select the **Print** button  to 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	Raman Shift Top (cm-1)	Absolute Height	Height	FWHM (cm-1)	Width (cm-1)	Wavelength Top (nm)	FWHM (nm)	FWHM (pixel)
1	16.418	-3.079	25116.531	23056.813	7.559	39.477	784.760	0.466	3.063
2	53.500	87.685	65931.625	49885.625	48.358	89.661	790.390	3.030	19.986
3	78.541	148.137	39340.823	4796.495	13.499	43.090	794.185	0.852	5.627
4	105.630	212.784	29680.146	16035.815	17.614	71.062	798.283	1.123	7.426
5	126.174	261.299	10104.308	255.517	6.725	16.447	801.387	0.432	2.861
6	131.875	274.683	9514.063	33.396	4.631	7.033	802.248	0.298	1.975
7	139.190	291.811	9584.286	75.083	3.969	9.355	803.351	0.256	1.698

12.5 Batch Re-Process

-  Batch Re-Process...
- Similar to **Experiment Setup**, but used to re-process spectra checked in the **Spectrum List Panel**.
- This function is different from other **Spectral Functions** in that it starts with the **Raw Data** blocks (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, while 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.
- Refer to Experiment Setup in Section 15.7 for details on processing features and a walk-through.



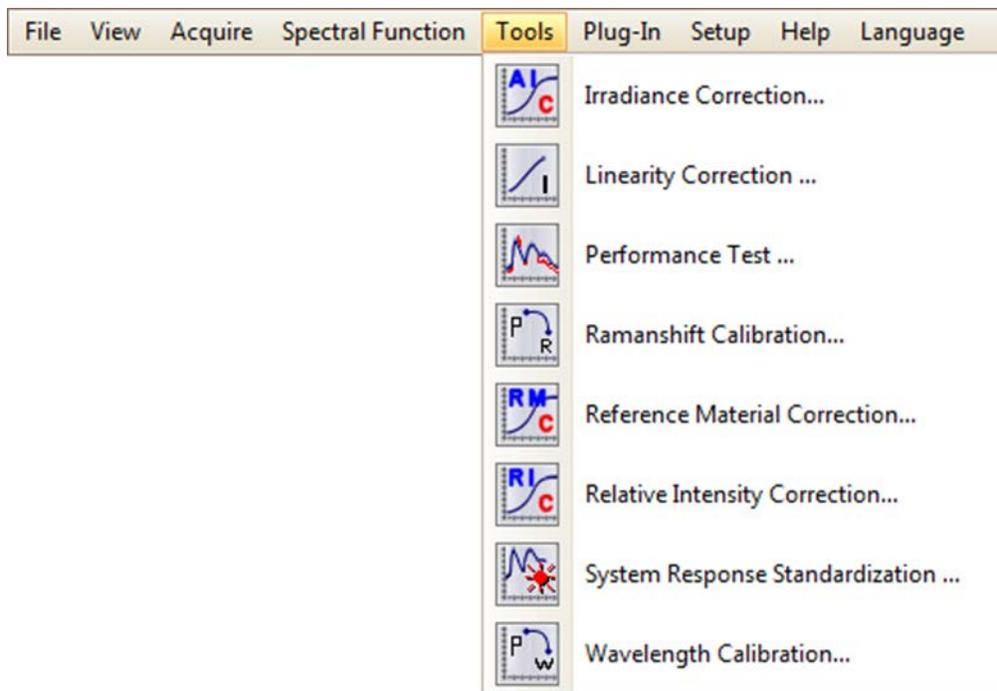
12.6 Spectra Math

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

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
- Enable this function in the **Plug-In Manager**. Refer to Section 24.10 for more details.

13 TOOLS



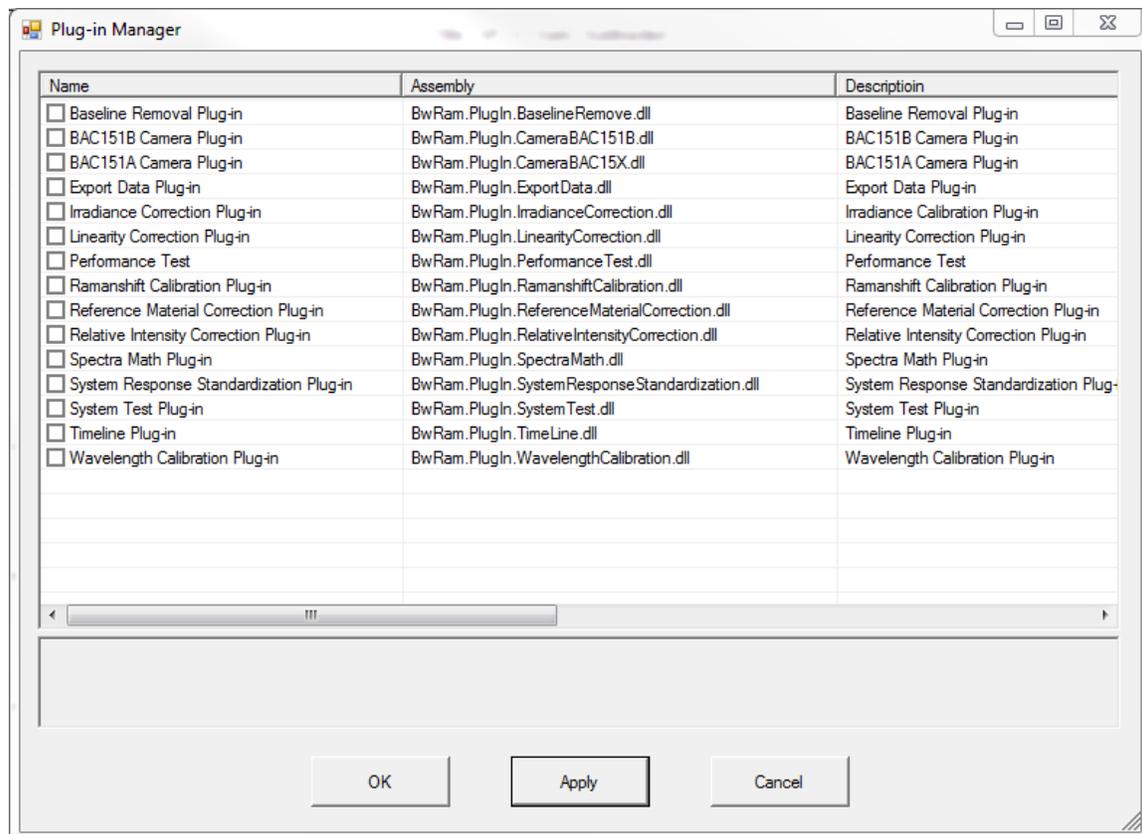
- This menu provides a set of instrument utility tools after being selected as Plug-Ins from the **Plug-In Manager**. Refer to Section 14.
- Please note that Linearity Correction, Raman Shift Calibration, System Response Standardization, and Wavelength Calibration are Factory functions and their results can only be written to the instrument's flash memory.
- **Irradiance Calibration:** Refer to Section 24.4
- **Linearity Correction:** Refer to Section 24.5
- **Performance Test:** For Raman instruments; provides a procedure for testing accuracy and repeatability of the hardware. Refer to Section 24.6
- **Raman Shift Calibration:** Refer to Section 24.7
- **Reference Material Correction:** Refer to Section 24.8
- **Relative Intensity Correction:** Refer to Section 24.9
- **System Response Standardization:** Refer to Section 24.11
- **Wavelength Calibration:** Refer to Section 24.13

14 PLUG-IN

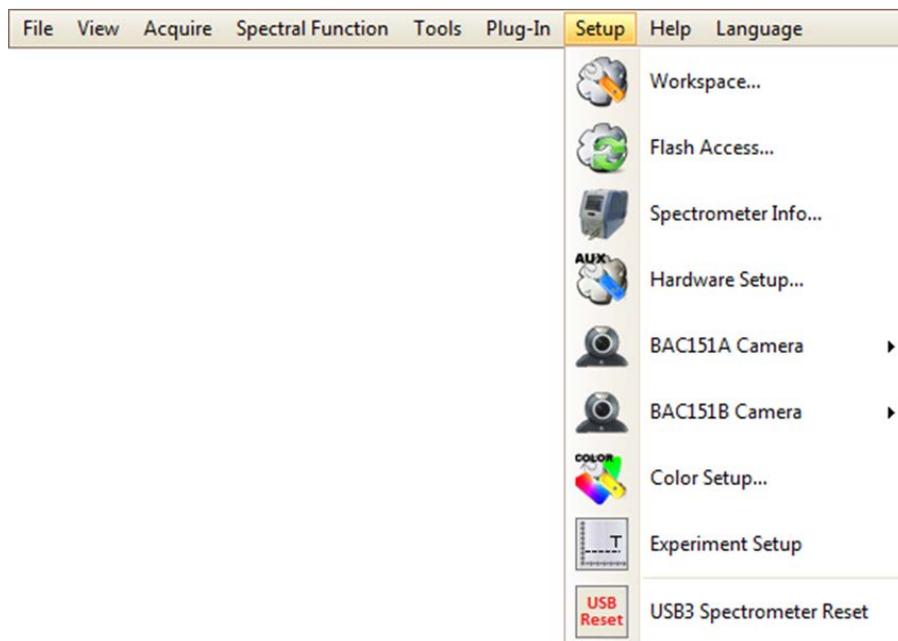


14.1 Plug-In Manager...

- Opens the **Plug-In Manager** 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.
- Refer to Section 24: **Plug-In Manager** for additional information about specific Plug-Ins.



15 SETUP

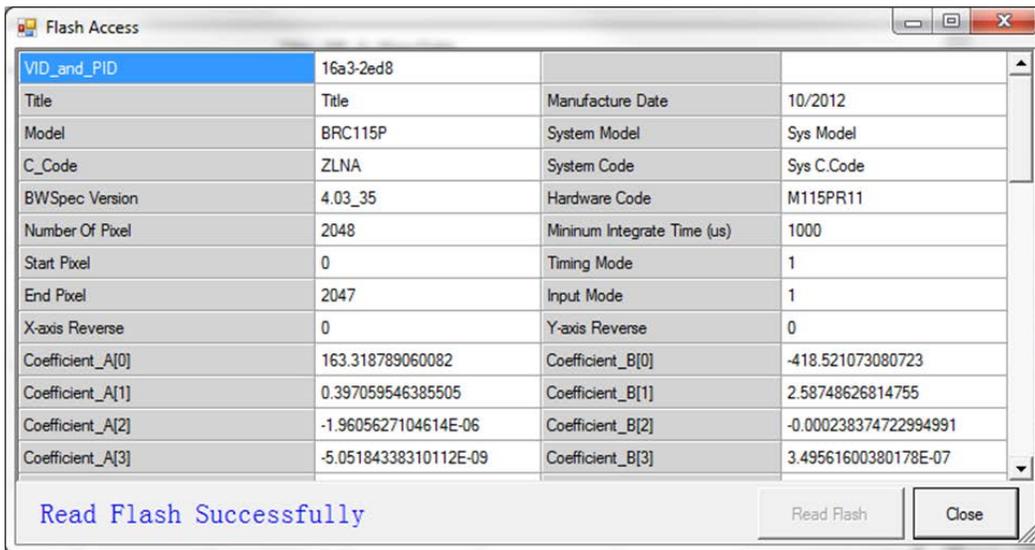


15.1 **Workspace**

-  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.

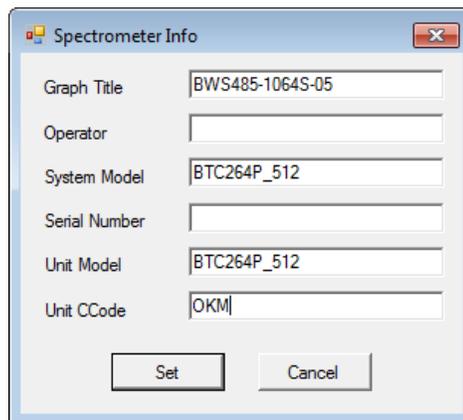
15.2 Flash Access...

-
- 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, including: wavelength calibration, display scales, and linearity correction.



15.3 Spectrometer Info...

-  Spectrometer Info...
- Opens a **Spectrometer Info** window which displays details of the spectrometer for the selected spectrum:
- Additional information can be input by the user for tracking purposes when printing/saving data.



15.4 Hardware Setup

-  Hardware Setup...
- This menu is active only when the BWSpec software is communicating with an instrument.
- Opens a **Hardware Setup** window which displays additional settings including Probe Setup and Auxiliary Port Control.
- Refer to section 23 for further details.

15.5 BAC151x Camera

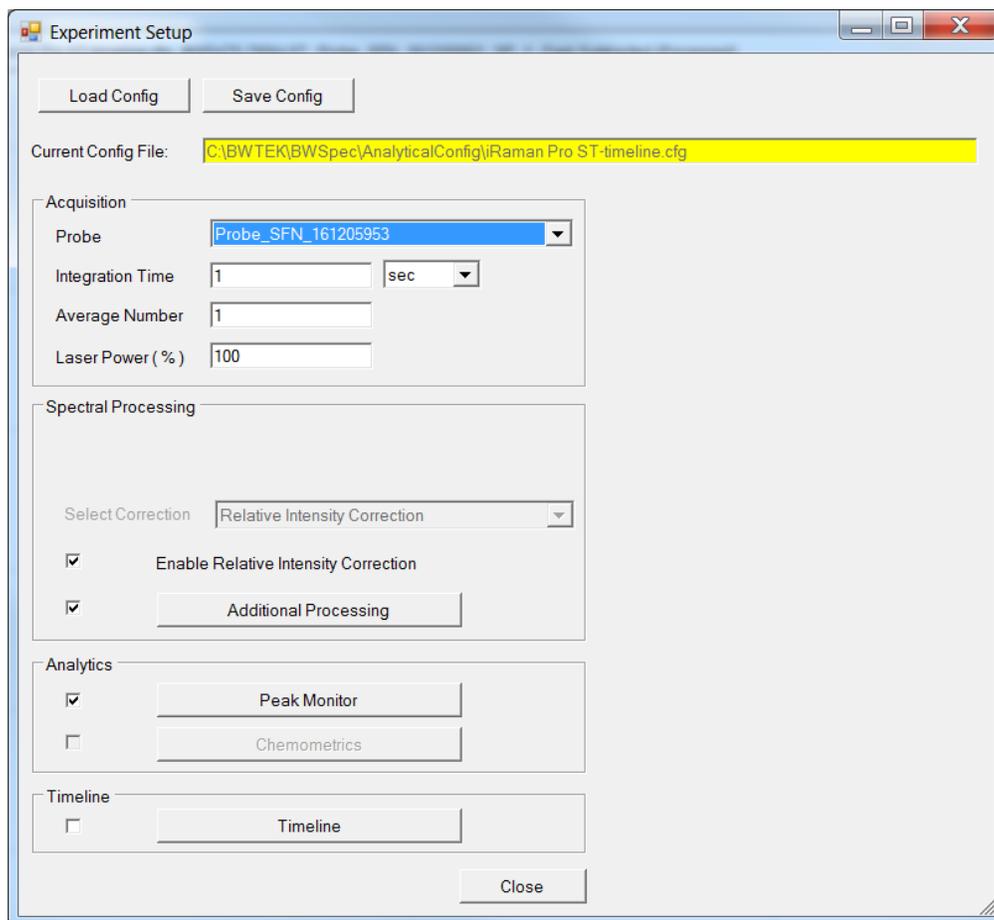
-  BAC151A Camera
-  BAC151B Camera
- Turns on the BAC151x camera
- BWSpec v4.11+ supports BAC151A rev A, BAC151A rev C and BAC151B.
- Refer to the BAC151x User Manual for details on installation and use.

15.6 Color Setup...

-  Color Setup...
- Opens a **Color Measure Setup** window.
- This feature is to be used with color measuring systems.
- Refer to Section 25: **Color Measurement** for more details.

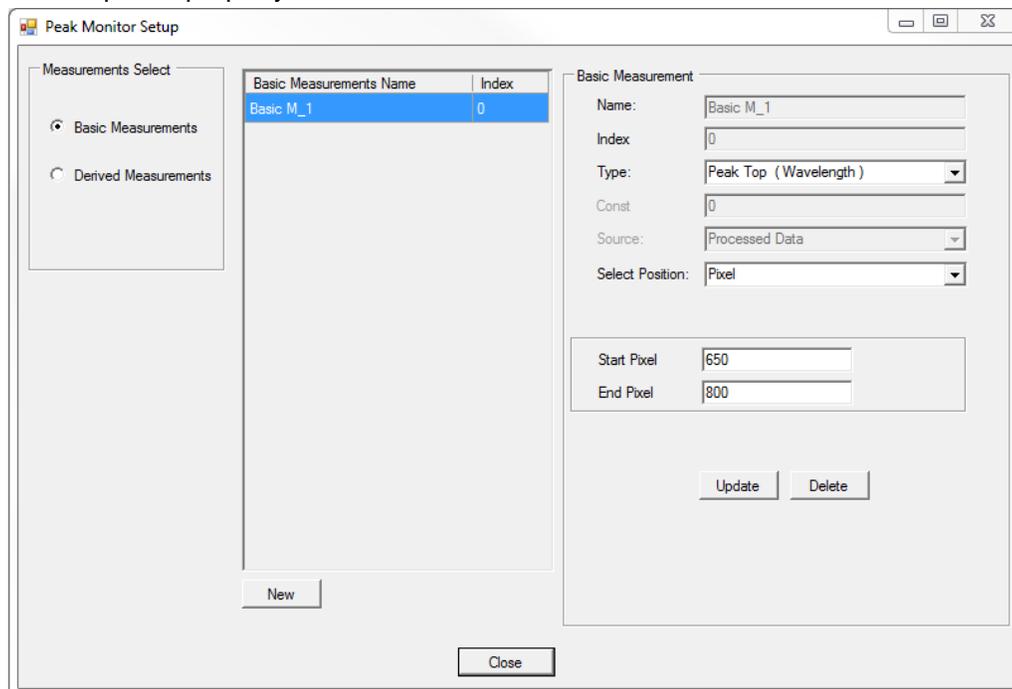
15.7 Experiment Setup

-  Experiment Setup
- Allows the user to create and save a set of parameters to define what and how to measure. This includes Acquisition, Spectral Processing, Analytics, and Timeline.
- Load Config load a previously saved Experiment Setup.
- Save Config saves the current Experiment Setup. Changes made to the current setup are lost unless they are saved.
- 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.
- Experiment Setup as viewed from the Raman Workspace:



- **Acquisition:**
 - Define the settings the instrument will use in each acquisition; including integration time and number of averages used for all instruments, also the laser power and probe used for Raman.
 - Allows for easy selection of probes 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 section 23.3 for more information on Probe Setup.
- **Spectral Processing:**
 - To perform predefined data processing
 - Options for intensity correction including: 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 or Dark Compensation is enabled, it is performed prior to any Spectral Processing 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 12 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

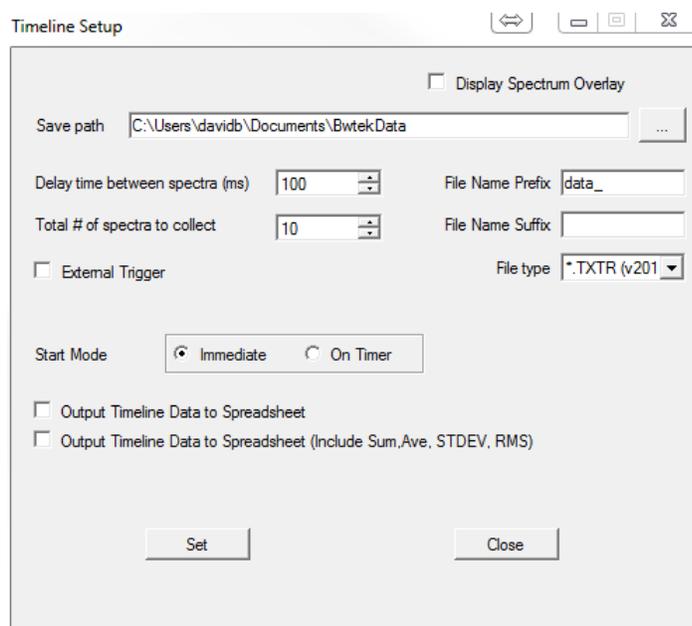


- Press the New button to add a new Measurement variable.
- The **Name** is to distinguish this measurement; this will be the title in Analytics.
- The **Index** will start at 0 and automatically increase for each additional measurement.
- The **Type** defines which peak parameter is being measured; Refer to Appendix B 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.

Sys Model,BRC115P		
Spectrum		Analytics
Data Source	Point	Time (sec)

- 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.
- Chemometrics Analytics are currently unavailable and the option is greyed out.

- **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 24.12 for more details.



Timeline Setup

Display Spectrum Overlay

Save path: C:\Users\davidb\Documents\BwtekData

Delay time between spectra (ms): 100

Total # of spectra to collect: 10

File Name Prefix: data_

File Name Suffix:

File type: *.TXTR (v201)

External Trigger

Start Mode: Immediate On Timer

Output Timeline Data to Spreadsheet

Output Timeline Data to Spreadsheet (Include Sum,Ave, STDEV, RMS)

Set Close

15.8 Raman Instrument Experiment Example:

- Find and measure multiple peaks using Probe and Relative Intensity correction and additional processing.
- 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**

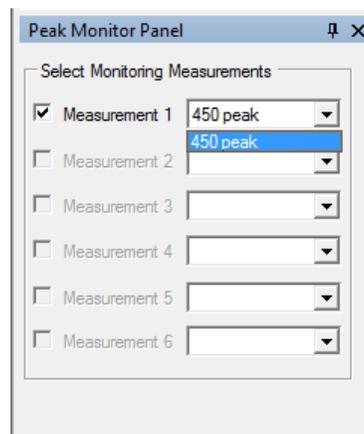
- Check the box next to **Timeline**, and then click the button to open the Timeline Setup window.
- Check the box **Display Spectrum Overlay** to have all the timeline acquisitions display in the main graph.
- Click the ... to select a save location for the new data.
- Select the **Delay time between 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**

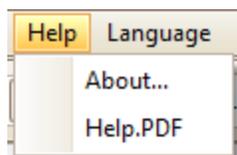
- Click the Timeline Acquisition button  to begin taking data.
- The top graph will display each spectrum as an overlay.
- The bottom graph will display the Peak Monitoring (Peak Height in this case) as a function of time. To toggle different peaks, go to the Peak Monitor Panel at the bottom right and 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.



15.9 USB 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.

16 HELP



- **About...**
- The **About** window provides B&W Tek. contact information
- BWSpec software version number.
- **Help.PDF**
- Opens the BWSpec User Manual as a .PDF document.
- This .PDF is also available in the BWSpec installation folder location (C:\BWTEK\BWSpec).

17 LANGUAGE

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



18TOOLBAR



Below is a brief description of the Toolbar icons. Many of these buttons can also be found in the Menu Bar under File, **View** and **Acquire**.

18.1 **Open**



-
- For opening files, saved in BWSpec, in the following formats:
- TXT File (*.txt)
- TXTR File (*.txtr)
- CSV File (*.csv)
- SPC File (*.spc)
- Spectral Signature File (*.sig)
- BWSpec Data File (*.BwRam)
- BWSpec Data BIN File (*.BwRamS)

18.2 **Save**



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

18.3 **Print**



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

18.4 Excel



- Exports the active/selected single spectrum from the Spectrum List Panel to Excel.
- Supported in all Excel versions.

18.5 Integration Time Control

Set Integration Time Time Unit Time Average



- Total Integration Time = Integration Time * Multiplier
- **Integration Time**
 - Exposure time setting for spectrometer.
 - Maximum Value is based on the Time Unit.
 - Minimum Value is based on the capability of the detector.
- **Unit**
 - Time unit for spectrometer acquisition time.
 - Set to minutes (min), seconds (sec), milliseconds (ms), or microseconds (µs). Microseconds (µs) is 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.

18.6 Acquire Control



- Refer to Section 11 **Acquire** for more information.

18.7 Reset Graph



- Resets 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.

18.8 **Clear Display**



-
- Removes all spectra in the graph and spectrum list panel.

18.9 **Display Scales**



-
- Opens the **Display Scales** Settings window.
- Refer to Display Scales in Section 10.4 View under **Menu Bar** for more details.

18.10 **BAC151x Control**



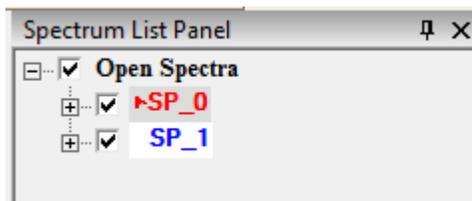
-
- Turn on the BAC151x Camera and opens a new View Window.
- The appropriate BAC151 A or B Plug-in must be enabled in Plug-In Manager, or else the button will be greyed-out.



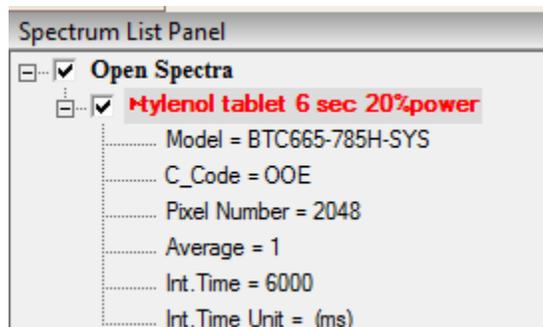
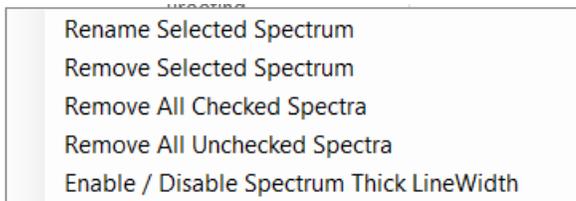
-
- Refer to the BAC151x User Manual for further details.

19 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 disc. 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 ↓ :



20 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.

Spectrum Information Panel	
Name	SP_1
DataSource	Spectrometer
Model	BRC115P
CCode	ZLNA
PixelNumber	2048
Average	1
IntegrationTime	1000
IntegrationTimeU (us)	
TimeMultiply	1
LaserWavelength	785
LaserLevel	0
ProbeName	
HadTakeRaw	True
HadTakeDark	True
HadTakeReferer	False
HadDarkCompen	False
Pretreat_0	
Pretreat_1	
Pretreat_2	
Pretreat_3	
Pretreat_4	
Pretreat_5	
Pretreat_6	
Pretreat_7	
Pretreat_8	
Pretreat_9	

21 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**.

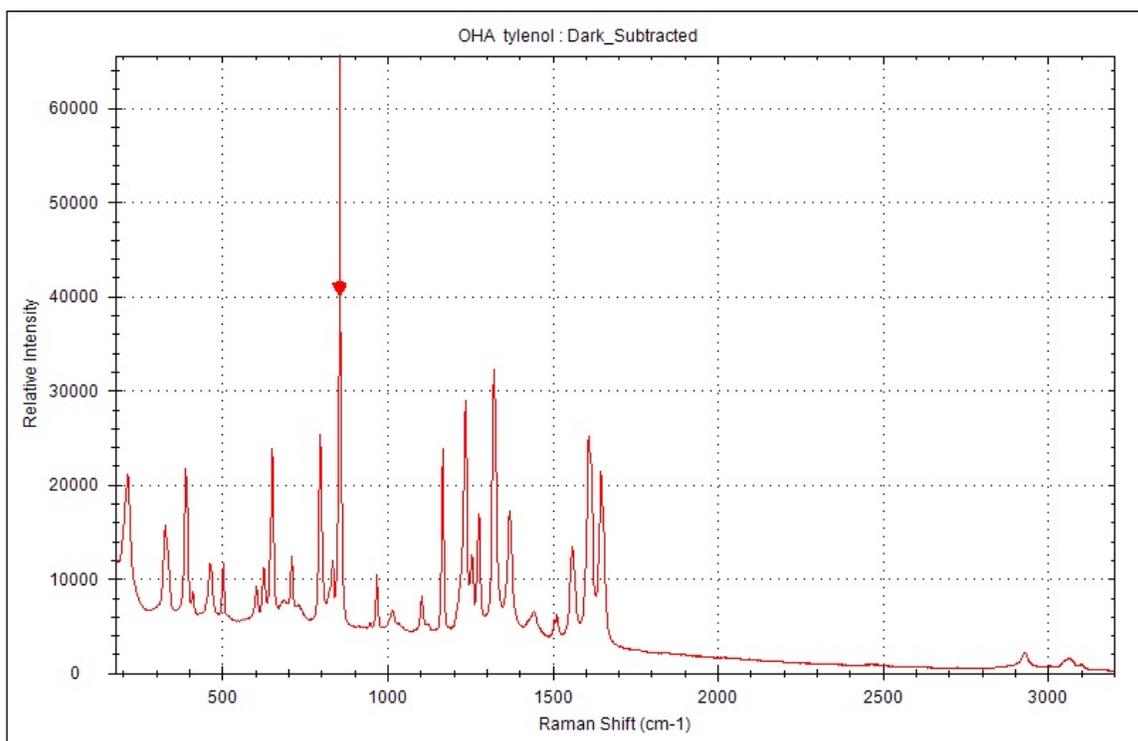
The screenshot shows the 'Spectrometer Control Panel' window. It is divided into several sections:

- Top Section:** Contains checkboxes for 'Enable Cursor' and 'Dual Chart'. A red box highlights these, with an annotation: 'Additional display options'.
- Display Options Section:**
 - X Axis Unit:** A list of radio buttons: 'Pixel', 'Wavelength (nm)' (selected), 'Wavenumber (cm-1)', 'Raman Shift (cm-1)', 'Wavelength linear (nm)', and 'Raman Shift linear (cm-1)'. A red box highlights this list, with an annotation: 'Select desired X-axis spectrum display mode.'
 - Y Axis Type:** A list of radio buttons: 'Raw Data' (selected), 'Dark', 'Reference', 'Dark Subtracted', 'Transmission/Reflection', 'Absorbance', and 'Absolute Irradiance'. A red box highlights this list, with an annotation: 'Select desired Y-axis spectrum display mode.'
- Acquire Control Section:** Contains checkboxes for 'External Trigger' and 'Auto Time'. A red box highlights these, with an annotation: 'Additional control options'.

At the bottom of the panel, there is a note: '**Available options may vary depending on your spectrometer or system**'.

21.1 **Enable Cursor**

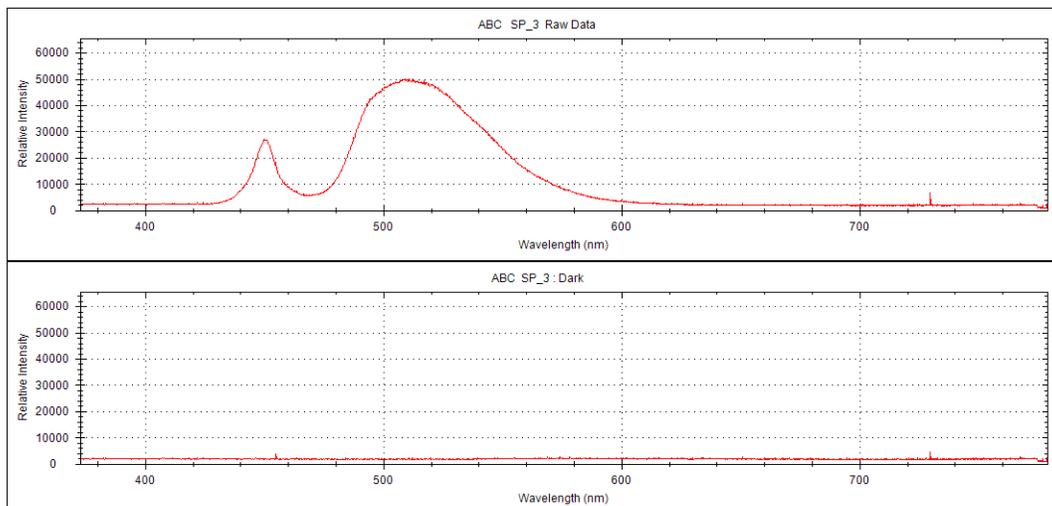
- This provides a vertical line on the graph which follows the mouse cursor. Information relating to the cursor location on the graph will be displayed at the bottom of the window in the status bar.
- *This feature can only be used on a spectrum that is displayed on the graph while the instrument is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



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

21.2 Dual Chart

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



21.3 X Axis Unit

- Changes the X-axis display mode.

21.4 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 (%):** $[(\text{Raw} - \text{Dark}) / (\text{Reference} - \text{Dark})] * 100$
- Absorbance:** $-\log(\text{Transmission}(\%) / 100)$
- Absolute Irradiance:** Shows the corrected spectrum when Irradiance Calibration is enabled.
- The spectrometer must have a valid Irradiance Calibration file.
- Refer to Section 24.4, Irradiance Calibration Plug-In for additional details.

Display Options

X Axis Unit

Pixel

Wavelength (nm)

Wavenumber (cm-1)

Raman Shift (cm-1)

Wavelength linear (nm)

Wavenumber linear (cm-1)

Raman Shift linear (cm-1)

Y Axis Type

Raw Data

Dark

Reference

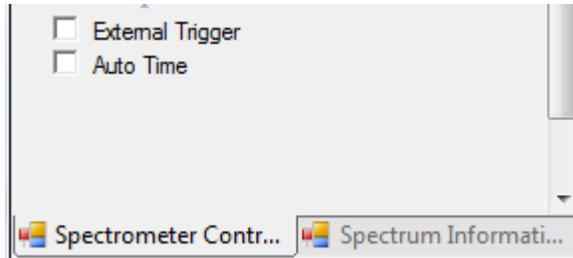
Dark Subtracted (Processed)

Transmission/Reflection

Absorbance

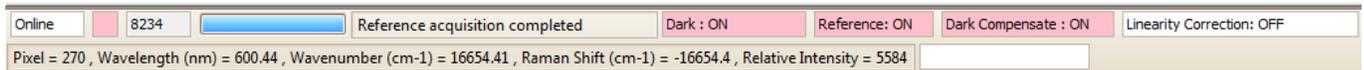
Absolute Irradiance

21.5 Acquire 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 Section 23 in Hardware Setup 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 become disabled until enabled again 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.

22 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:

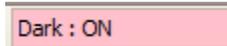


- **Acquisition status bar**



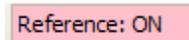
- Increases as the scan progresses
- Useful for long integration times or multiple averages.

- **Dark Array Status**



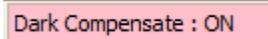
- Gives status if a Dark Scan has been taken and saved into the Dark Array for the “active” spectrum.

- **Reference Array Status**



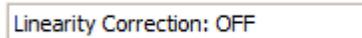
- Gives status if a Reference Scan has been taken and saved into the Reference Array for the “active” spectrum.

- **Dark Compensate**



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

- **Linearity Correction**



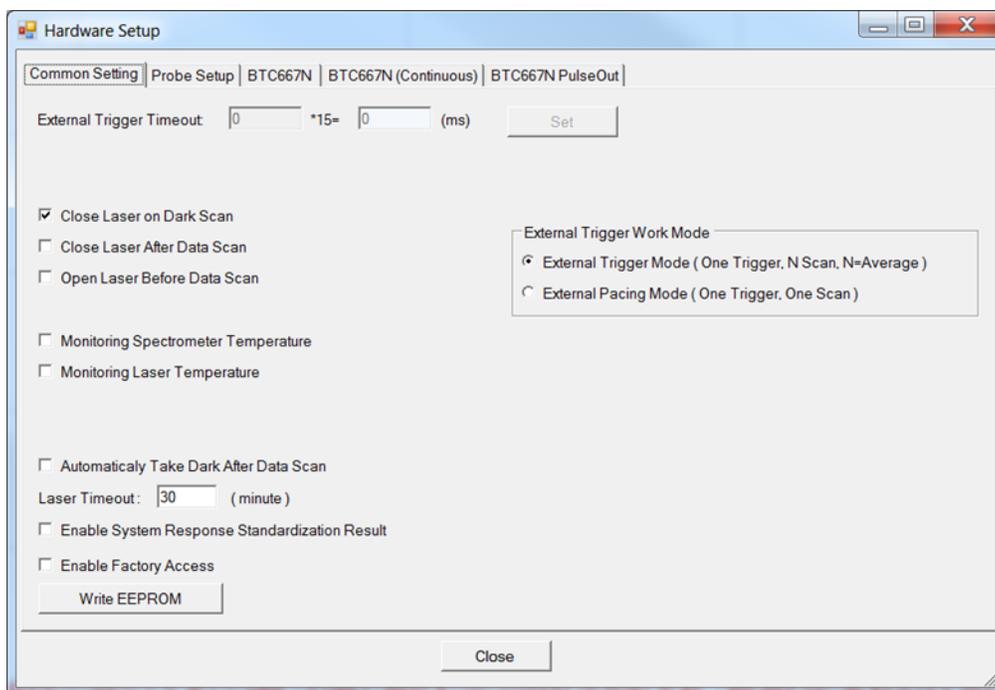
- Gives status of the **Linear Correction** function

23 HARDWARE SETUP

The following is an explanation for different features within Hardware Setup. Hardware Setup is only accessible from the Setup menu when BWSpec is communicating with a B&W Tek Spectrometer. Some features are model specific.

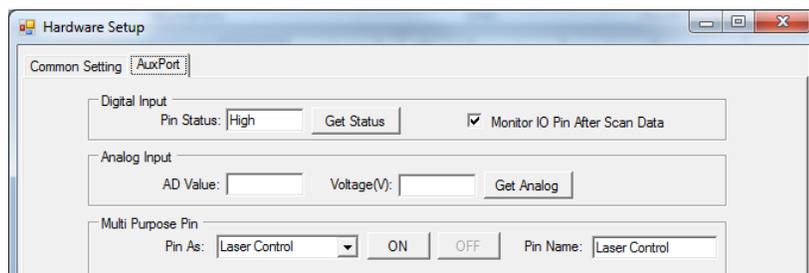
23.1 Common Setting

- Not all features listed will work with specific spectrometer models.
- Check your product's User Manual for details relating to additional controls.



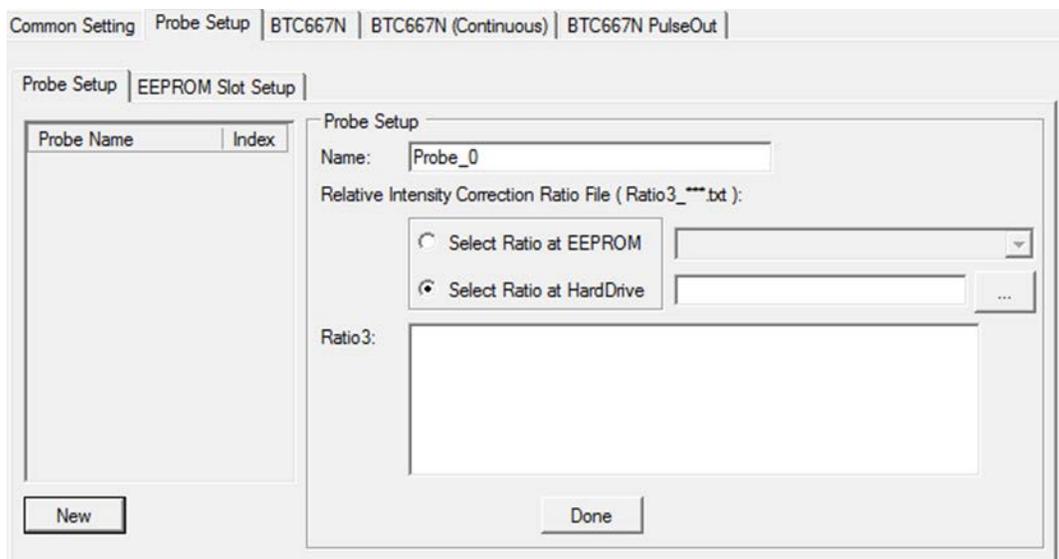
23.2 AuxPort

- Not all features pictured will work with all spectrometers. Check the product's User Manual for details relating to AuxPort Controls.



23.3 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 at <http://bwtek.com/support/>
- The Ratio3 information will now be displayed, Click **Done** to accept.



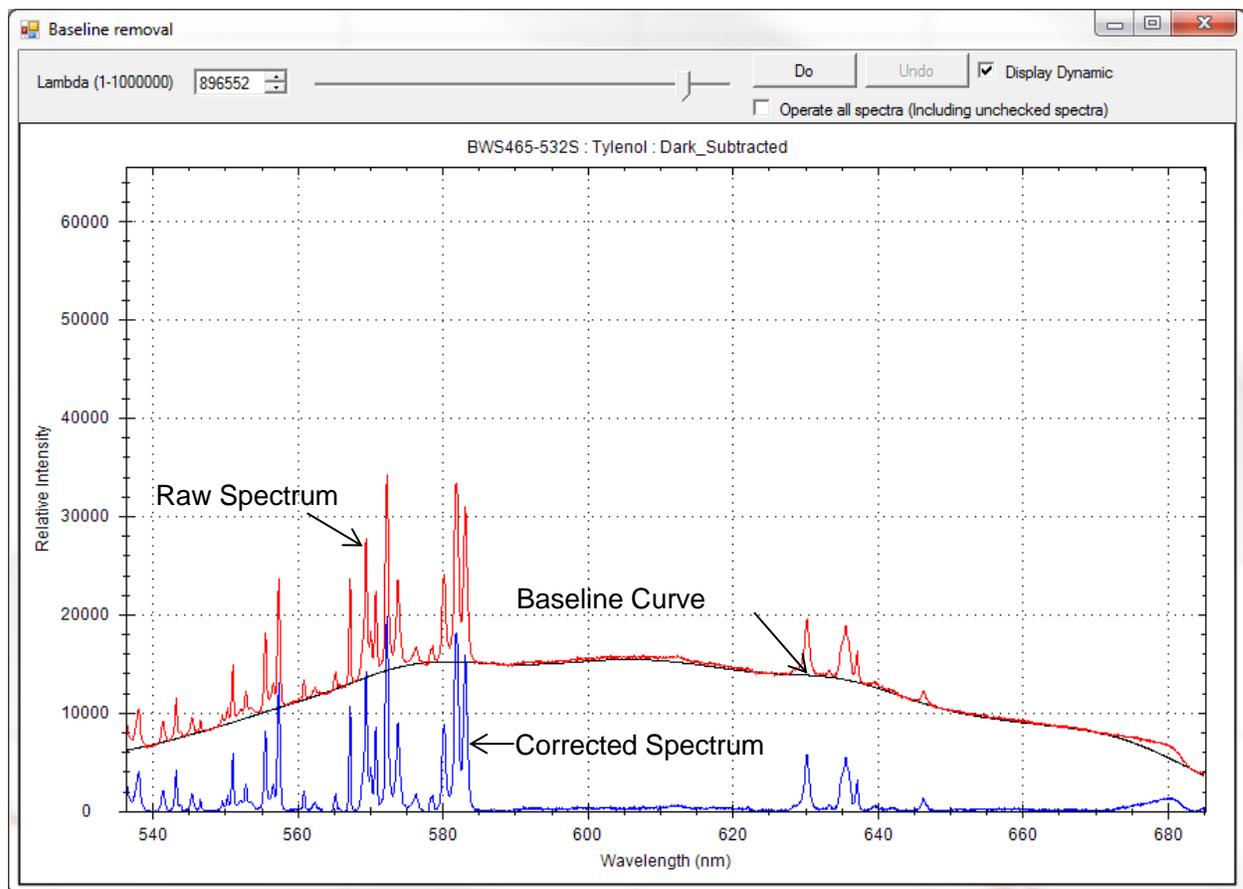
- You may use the Ratio3 created at the factory or you can create your own. Experienced customers can refer to Section 24.9 for more details. The appropriate Standard Reference Material is required to create a good Ratio3 correction file.
- EEPROM Slot Setup: Do not use this feature.

24 PLUG-IN MANAGER

The following is an in-depth explanation for each Plug-In function and its location on the Menu Bar.

24.1 *Baseline Removal Plug-in*

- 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.
- Location: Menu Bar → Spectral Function
- 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.



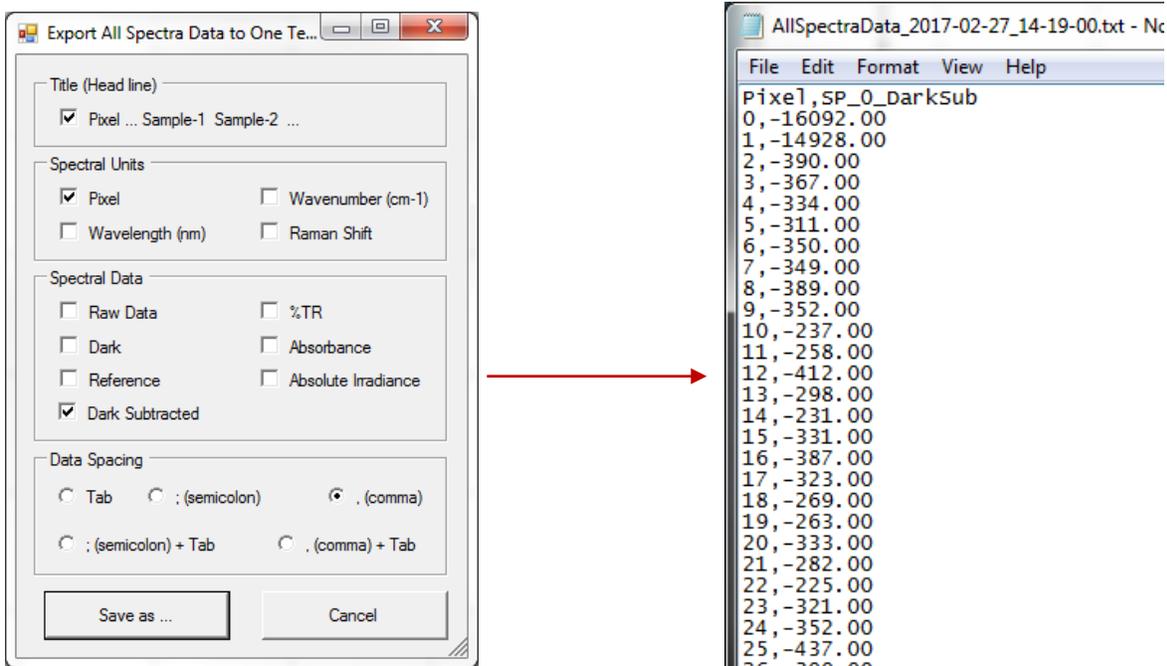
24.2 BAC151x Camera Plug-in

- The BAC151x Camera Plug-in is used to turn on the camera.
- 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.

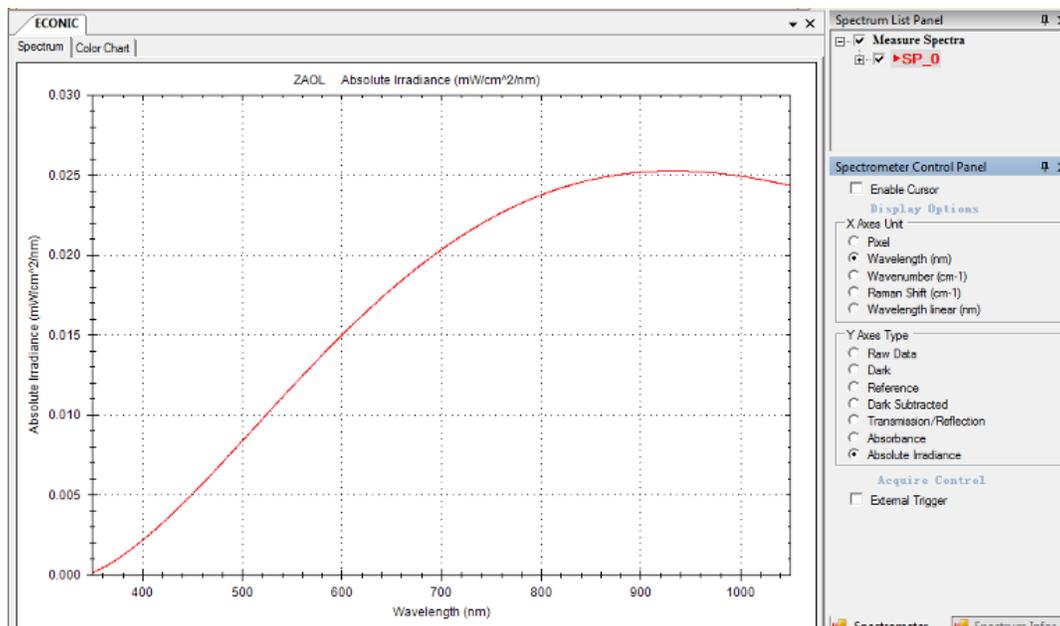
24.3 Export Data Plug-in

- 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**.
- Select the data information to be exported, and click **Save As**.
- All selected Spectra will be exported and saved to a text file.



24.4 Irradiance Calibration Plug-in

- This option is available only when in the BWSpec Workspace. Irradiance Calibration can be conducted by B&W Tek. using NIST-Traceable Irradiance Standards and calibration setups, if so desired. Irradiance Calibration is an option that can be ordered upon placing a spectrometer order, or through a service request.
- Location: Menu Bar → Tools
- **How to apply an Irradiance Ratio File**
 - Go to Setup > Experiment Setup
 - Under Spectral Processing, select Irradiance Calibration under “Select Correction”
 - Under that, click Ratio File button and find the appropriate Ratio file. Click OK.
 - Enable the Checkbox next to Enable Irradiance Correction to enable the process.
 - Save the configuration file and click Close when done.
 - Click “Absolute Irradiance” on the Spectrometer Control Panel. The Absolute Irradiance curve will show on the display after a scan has been taken.
 - You may need to adjust the X-axis and Y-axis scales in order to get a suitable display scale.

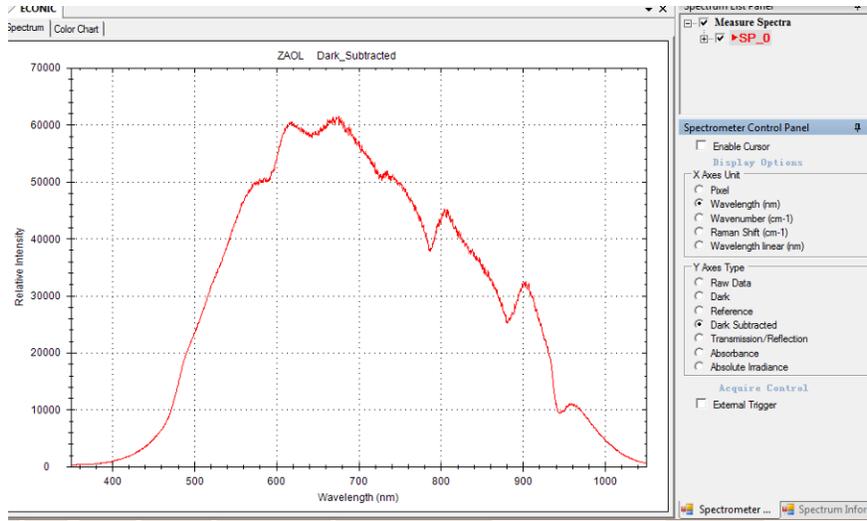


- **How to Conduct Irradiance Calibration and create a ratio file**

WARNING: This section is for advanced users only.

- In order to conduct an Irradiance Calibration, you must first have a NIST Traceable Lamp Source with certified values which cover the spectral range you will be calibrating your spectrometer to and the .DAT file that accompanies your lamp.
- It is also necessary to have the correct input optics for your spectrometer to collect the light, such as a fiber and an integrating sphere.
- The spectral irradiance calibration will allow a spectrometer to convert spectral measurements to absolute spectral irradiance measurements in units of light power in $W / [cm^2 \cdot nm]$, $mW / [cm^2 \cdot nm]$ or $\mu W / [cm^2 \cdot nm]$. Alternatively, a spectral irradiance calibration can be used to calibrate the spectrometer for emissive photometric measurements, such as for the color of an emissive source (for example, LED).
- Your setup conditions, distance from source, and lamp current must be as close as possible to what your NIST Certificate states in order to conduct a successful calibration. 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):

- Adjust the integration time so that the maximum spectral response is just below the spectrometer's saturation level against the certified lamp at a specified distance. Stop the acquisition and freeze all physical setup with minimal disturbance.
- **Step 1:** Cover your light input aperture so that no light is gathered by your setup 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.



- From the Menu Bar, select **Tools** → **Irradiance Calibration**.
- **Step 2:** 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 manner in which BWSpec can read it. Please refer to Section 27 **“Definition of Irradiance Data File Format”** for formatting info.

Create Irradiance Correction Ratio File

Step 1: Turn off light, take a dark scan, then turn on light, take a single raw data scan.

Step 2: Please Select the Location of the Lamp File.

Lamp Data Info: Start WL WaveLength (nm) Absolute Irradiance
 End WL
 Inc WL

Step 3: Input Distance and unit of Lamp Data. Distance (cm) Unit

Step 4: Select Curve Fit Method. Regressions Interpolations Order

Step 5: Select Data. Use Current Spectrum

Step 6: Input Distance between the lamp and the spectrometer. (cm)

Step 7: Input Transmittance of Neutral Density Filters: % (Neutral Density Filters

Step 8: Set ratio file name
 Set ratio file path

Step 9: Create ratio file

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

24.5 **Linearity Correction Plug-in**

- 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 in order for the Linearity Correction Coefficients to be saved into device memory. "Linearity Correction" is an upgrade option to be ordered when purchasing the spectrometer or through a service request.
- **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 Option → Linearity Correction. The linearity correction window will appear. Follow Step 1 through Step 9 instructions in the window to proceed. See the next page.

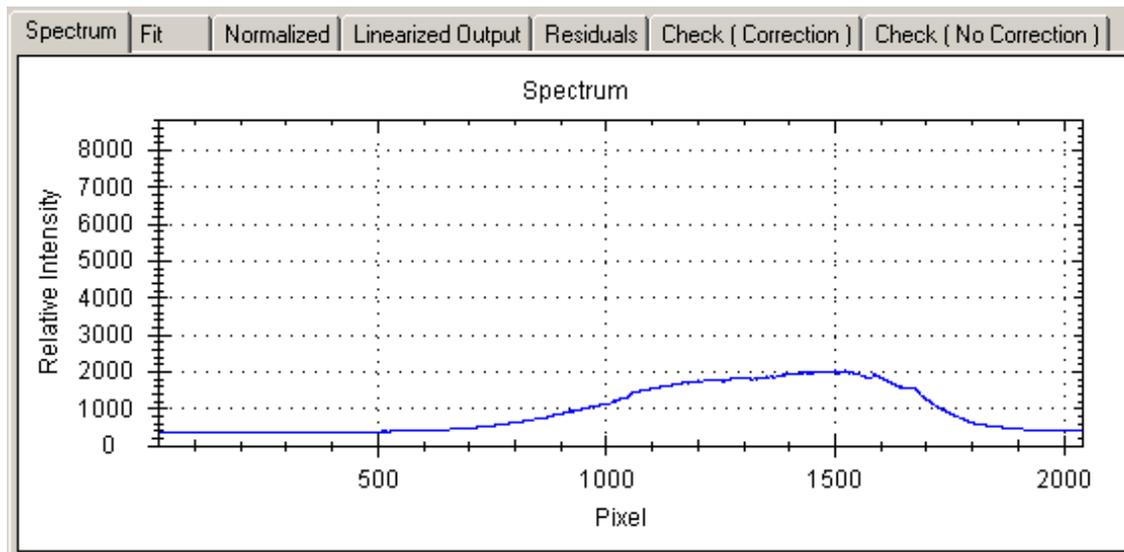
Adjust starting integration time, multiplier, and average. Peak intensity should be around 2,000 counts.

Enable Boxcar smoothing during correction process.

Display active Linearity Correction Coefficients saved to the flash.

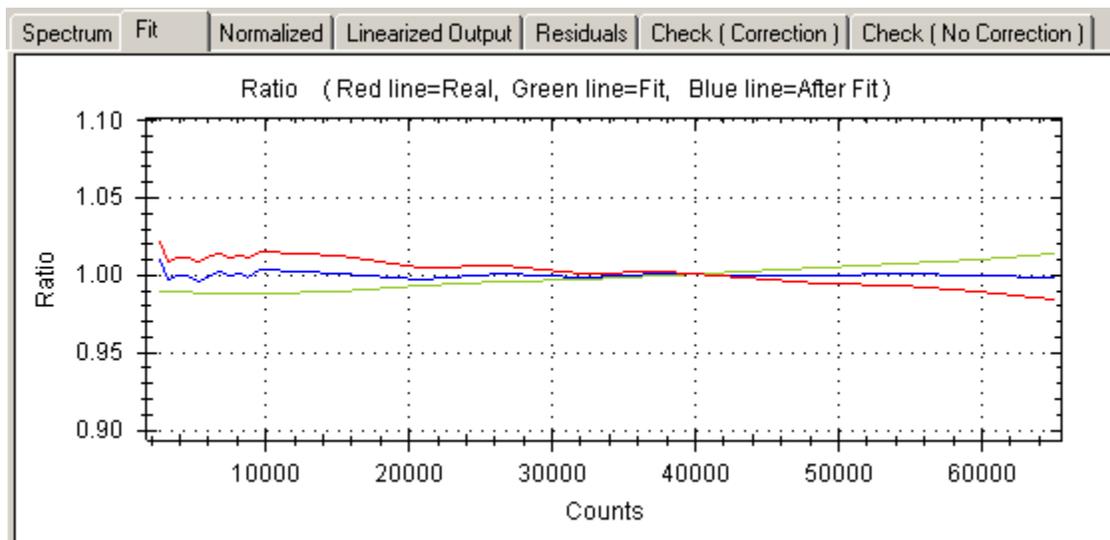
Select from 4-7 order fitting curves and calculate Linearity Correction Coefficients

Print Linearity Correction Report



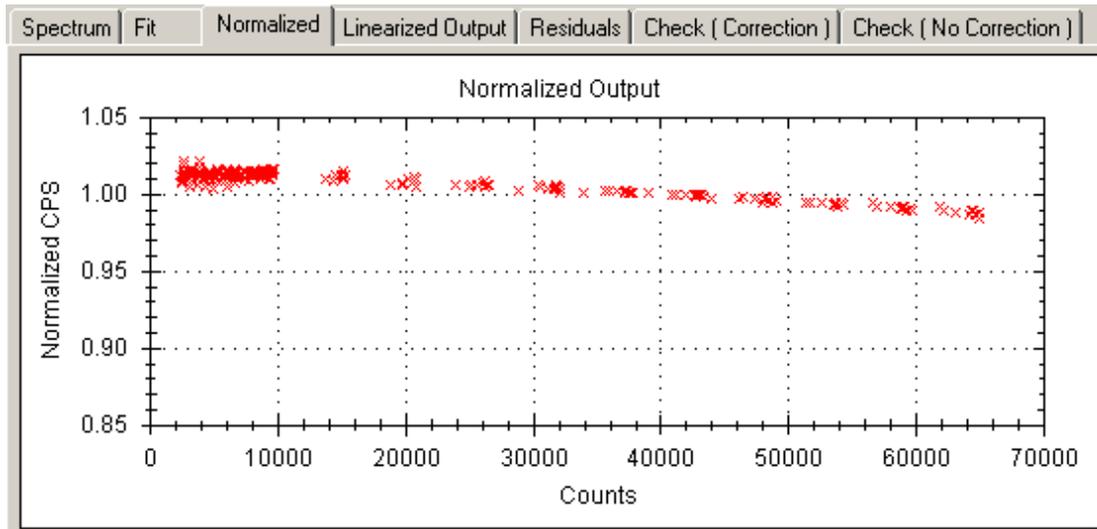
- **Spectrum**

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

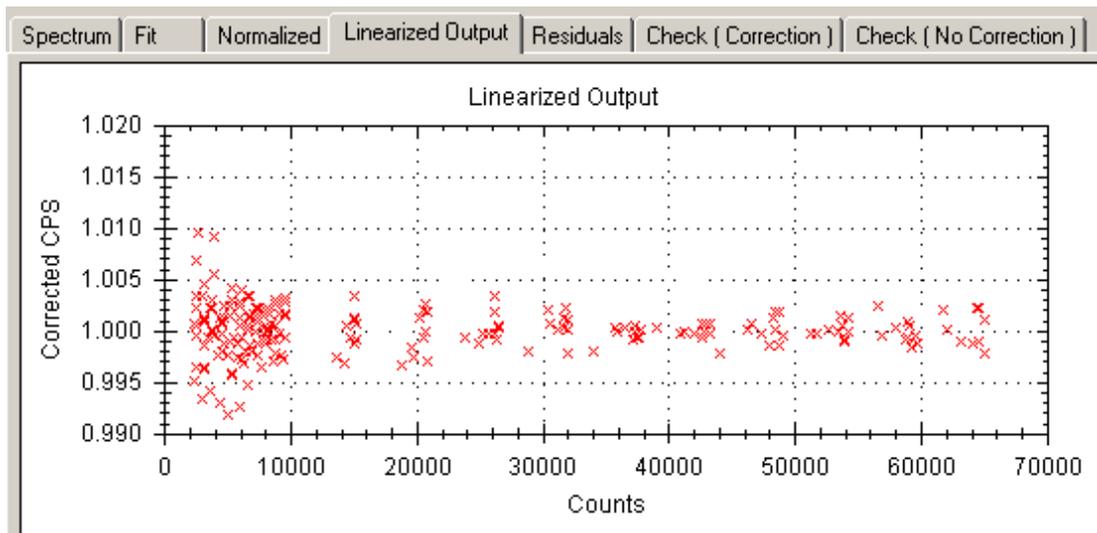


- **Fit**

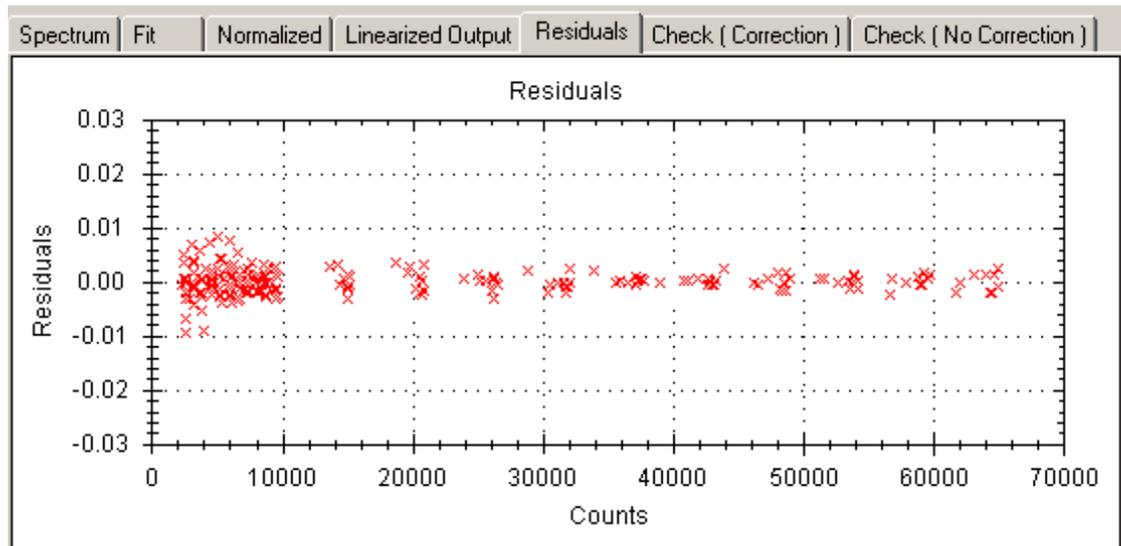
- Displays the fitting curve of the correction based on the Order (Step 9).
- Red is the Original, Green is the Fit curve, and Blue is the Corrected



- **Normalized**
 - Displays the output before correction

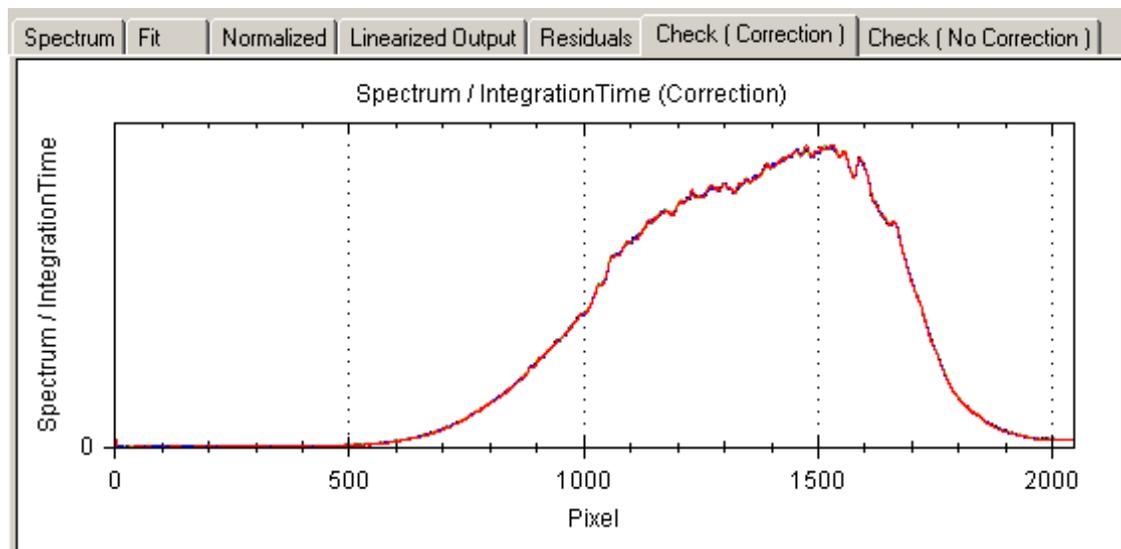


- **Linearized**
 - Displays the output after correction.



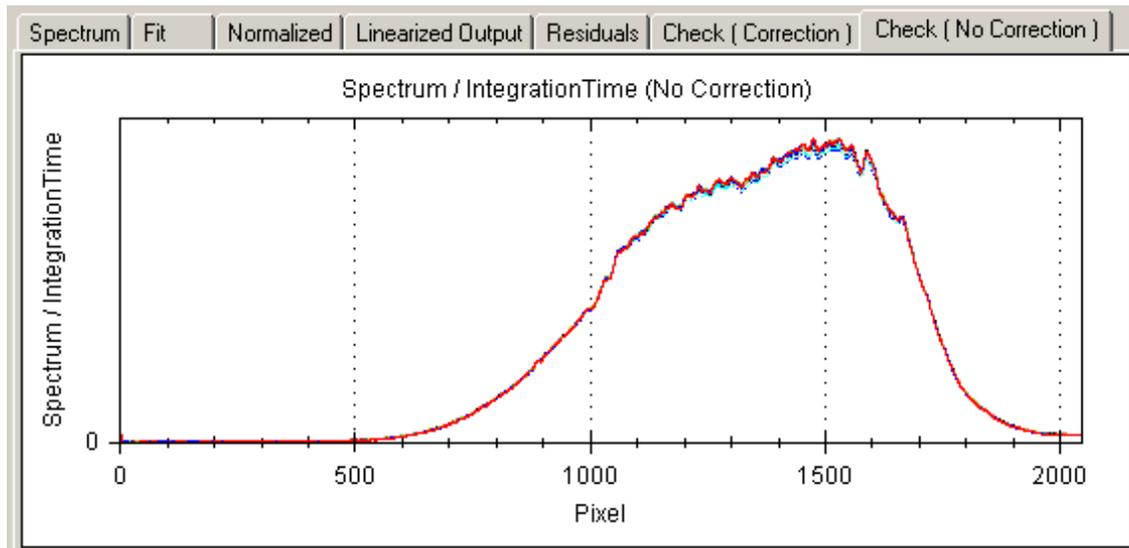
- **Residuals**

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



- **Check (Correction)**

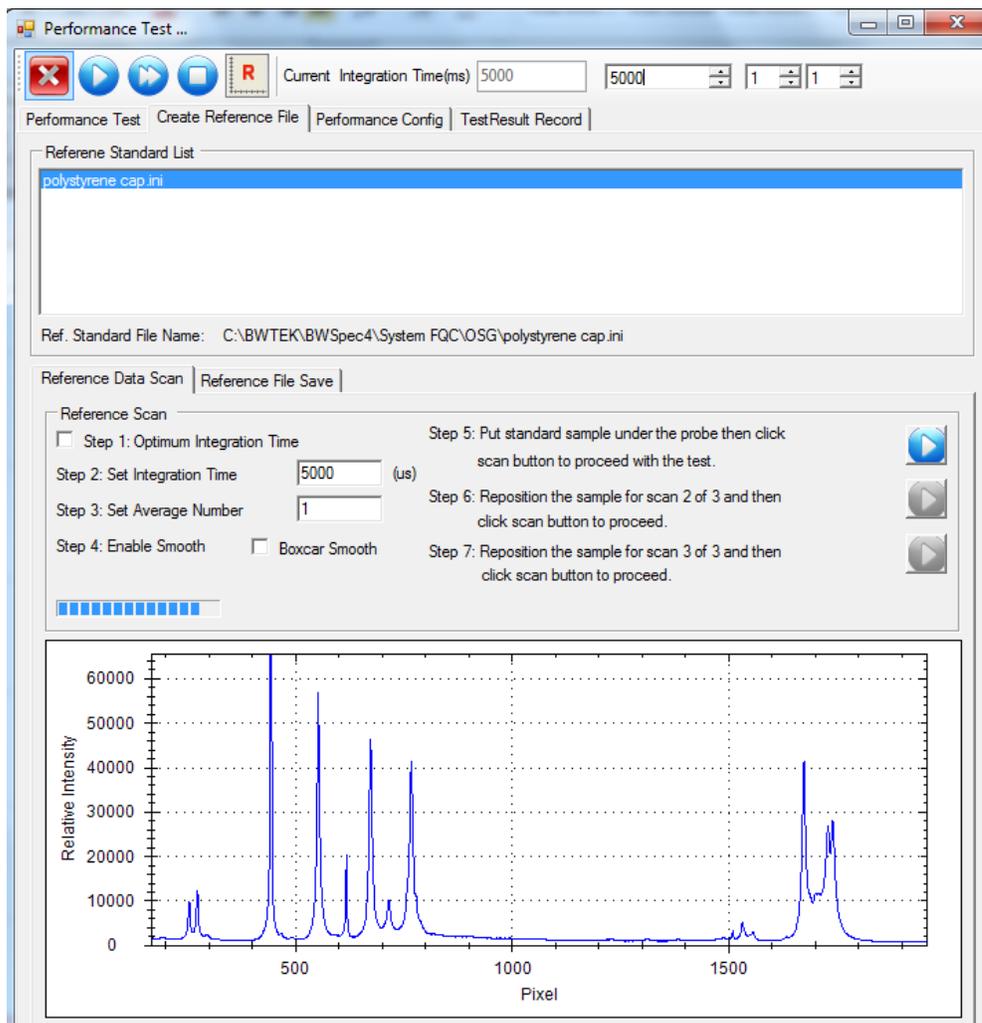
- Displays the corrected Spectrum/Integration vs Time graph

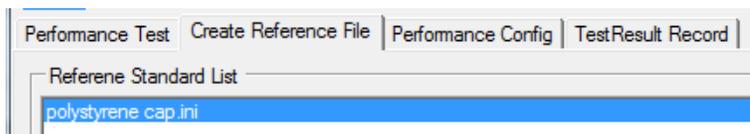


- **Check (No Correction)**
 - Displays the uncorrected Spectrum/Integration vs Time graph.
- **Note:** Once the Flash is re-read, the current active Linearity Coefficients will be lost. Linearity Correction conducted by the factory will have the coefficients saved in Flash.
- **Note:** The key for a 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.

24.6 Performance Test Plug-in

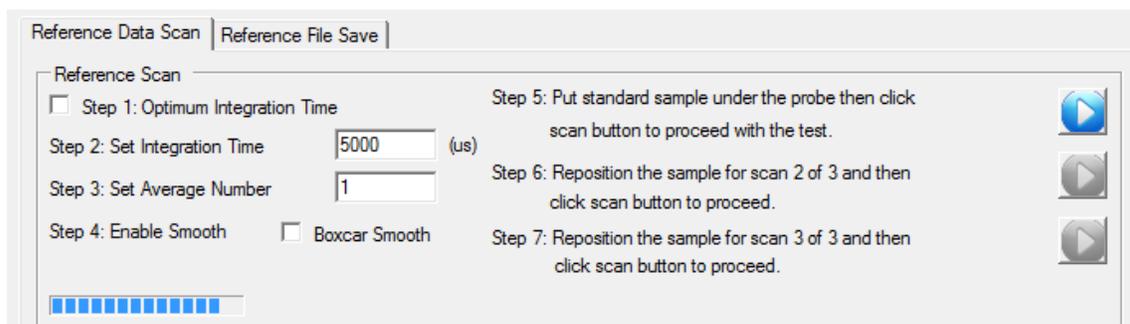
- The Performance Test is a procedure that evaluates a Raman instrument's performance with regards to accuracy and repeatability of instrument readings. This feature is available when the software is communicating with a Raman instrument.
- The performance test will validate a single peak of a reference standard spectrum. It will check if the peak is within acceptable limits: the peak's signal must be within 30% of the factory settings and the peak's shift must be no more than one pixel off of the factory settings, where the factory setting is a predefined reference standard spectrum.
- Reference files are user created and should be made as soon as possible with the new unit. The performance test should be performed on a regular basis to ensure consistency in the performance and operation of the instrument.
- Location: Menu Bar → Tools





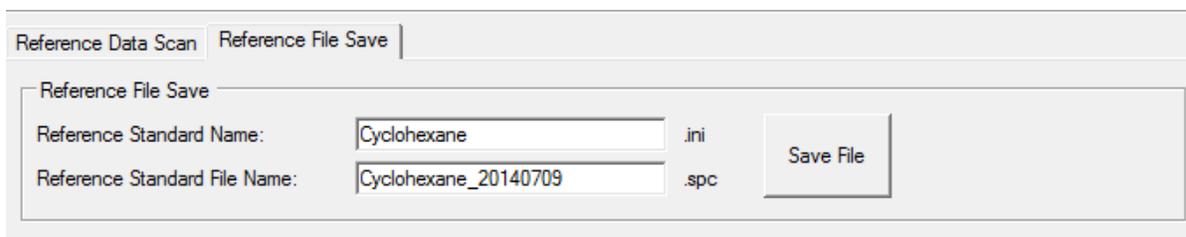
- **Create Reference File**

- A new reference file may be created in this tab.
- The user is responsible for providing a Raman-active sample with distinguished peaks.
- Use the Acquire Spectrum buttons and the Integration Time at the top of the window to determine the correct values for the Reference Data Scan. Make sure the peaks are visible and distinguishable. By selecting Optimum Integration Time, the system will determine the best integration time to use.



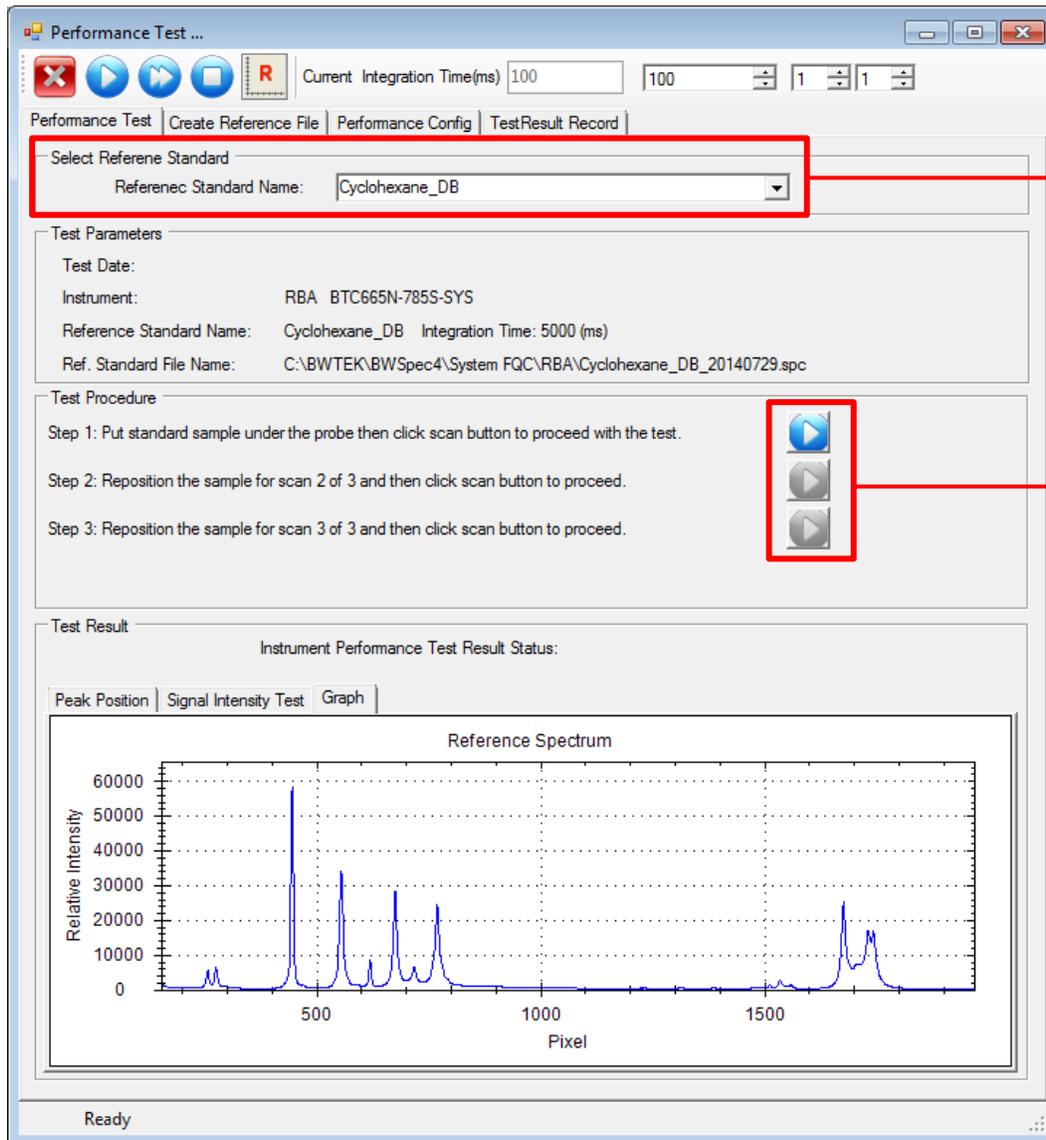
- **Reference Data Scan**

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



- **Reference File Save**

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



Select a pre-configured reference standard

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

- **Performance Test**

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

- **Select Reference Standard**

- Use the same reference standard that is going to be used as a sample in the performance test. The default is polystyrene.

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

Peak Position	Signal Intensity Test	Graph
Peak Position Test Status: Passed		
Reference Peak Position (Pixel):	447	
Measure Peak Position (Pixel):	446	HQI: 96.11
Peak Shift (Pixel):	1.0	
Test Acceptance Limits:	+/- 1 (Pixel shift)	Minimum HQI: 85
Spectra File:	C:\BWTEK\BWSpec4\LogData\Perftest\RBA\2014\PT_20140806105349.spc	
Results File:	C:\BWTEK\BWSpec4\LogData\Perftest\RBA\2014\PT_20140806105349.ptf	

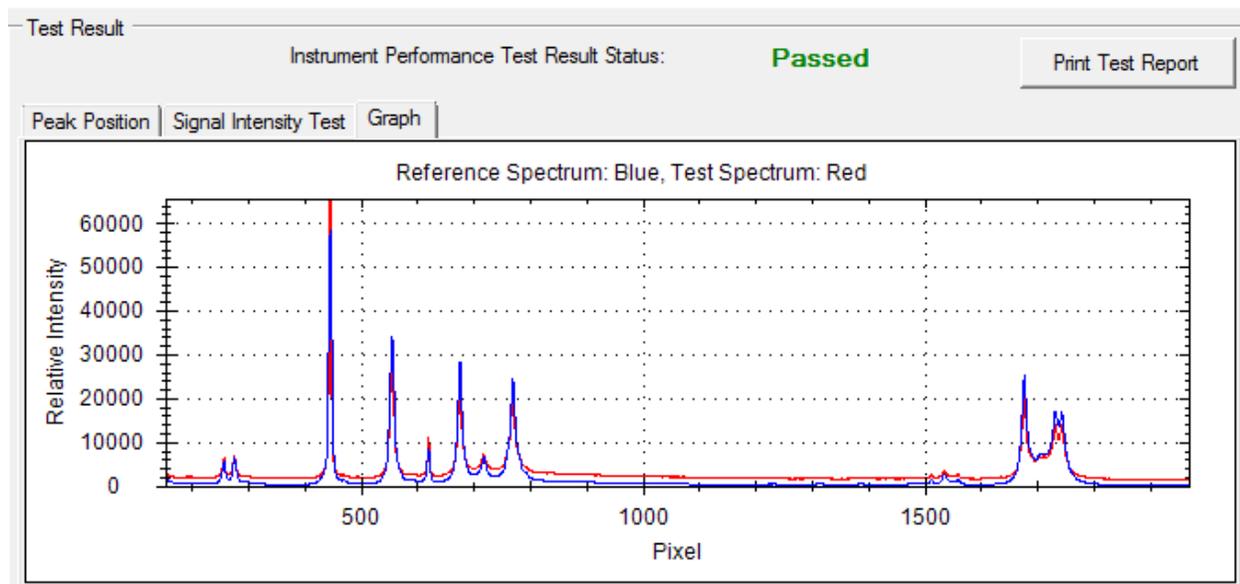
- **Peak Position**

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

Peak Position	Signal Intensity Test	Graph
Signal Intensity Test Status: Passed		
Reference Peak Signal Intensity:	58370	
Measure Peak Signal Intensity:	65535	
Test Acceptance Limits:	Minimum : 40859	Maximum : 65535

- **Signal Intensity Test**

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



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

Performance Test | Create Reference File | Performance Config | TestResult Record

Performance Test Records

Operator: All | Year: All | Mon: All | Day: All

PT_20140625082739.ptf
 PT_20140625082940.ptf
 PT_20140625083013.ptf
 PT_20140625083030.ptf
 PT_20140625083132.ptf
 PT_20140709134624.ptf

Record Information

Performance Test Result : **Passed** Print Test Record Report

Test Date: 2014-07-09 13:46:24

Instrument: OSG BTC665N

Reference Standard Name: Cyclohexane Integration Time: 5000 (ms)

Ref. Standard File Name: C:\BWTEK\BWSpec4\System FQC\OSG\Cyclohexane_20140709.spc

Spectra File: C:\BWTEK\BWSpec4\LogData\Perftest\OSG\2014\PT_20140709134624.ptf

- **Test Result Record**
 - The spectrum is stored in a Grams SPC data file format (*.spc), while the test results are saved in a BWTek proprietary binary file format (*.ptf).
- **Performance Test Records**
 - The test records may be searched by Operator or by Date
 - Select the file to view its information
- **Record Information**
 - The results of the Performance test are displayed
 - Click the **Print Test Record Report** to view and print the record.

Performance Test | Create Reference File | Performance Config | TestResult Record

Config

Xaxis_Min (RamanShift)	<input type="text" value="200"/>	(cm-1)
Xaxis_Max (RamanShift)	<input type="text" value="2800"/>	(cm-1)
Peak Threshold	<input type="text" value="1500"/>	(counts)
Laser Level (%)	<input type="text" value="100"/>	
Standard HQI	<input type="text" value="85.00"/>	
Standard Peak Pixel Shift	<input type="text" value="1"/>	
Standard Peak Intensity High Ratio	<input type="text" value="1.30"/>	
Standard Peak Intensity Low Ratio	<input type="text" value="0.70"/>	

Enable Change Config

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

24.7 Raman Shift Calibration Plug-in

This Plug-In is not intended to be used by end users. Raman Shift Calibration must be conducted by B&W Tek, 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.

24.8 Reference Material Correction Plug-in

- In applications such as diffuse reflectance measurements, a certified reflectance standard is often used to serve as a reference. The %R values throughout the measurement range are then calculated by using ratios with respect to the reference in a relative sense. With the available certified %R values, the BWSpec software can calculate the “absolute reflectance” against the reference.
- Location: Menu Bar → Option
- The following is a table of typical %R values obtained using a certified white PTFE type material spectral reflectance standard (B&W Tek model number SRR-1.25-99 or SRR-2.0-99).

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

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

$$\%Rs \text{ (non-correction)} = (\text{Sample intensity}/\text{Reference intensity}) * 100.$$

After reference material correction:

$\%Rs \text{ (absolute)} = \%Rs \text{ (non-correction)} * \text{Certified \%R value}/100$ where all values are calculated at given wavelengths across the calibration wavelength range.

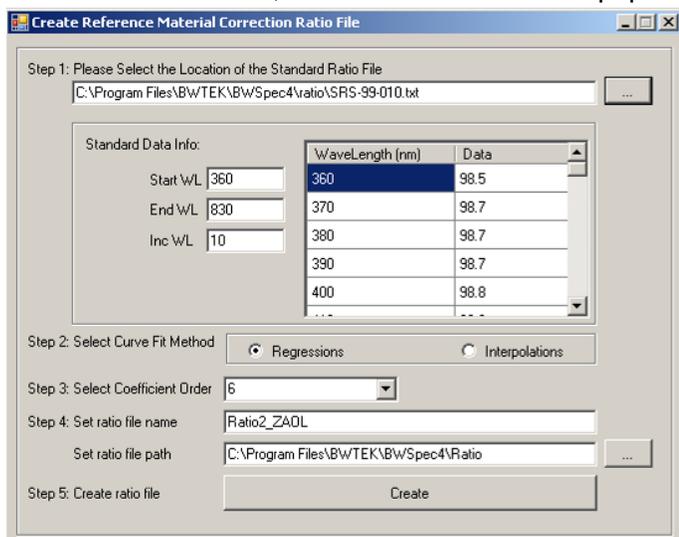
- **Generate Reference Material Correction Ratio File**

- This section is for advanced users only.

- Collect a spectrum using reference materials.

- Select **Option** → **Reference Material Collection**.

- Click  and browse to locate the “Reference Material ratio.txt” file. You will be directed to the default path where this file is stored: C:\Program Files\BWTEK\BWSpec4\ratio\. This file contains the certified values of spectral reflectance over the wavelength range of interest. After the file is loaded, the standard data will be populated.



- Follow the steps stated to fill out the parameters for the correction. The default ratio file name is Ratio2_C-code.

- Click **Create** to generate a Ratio2 file.

- **Enable Reference Material Correction Files.**

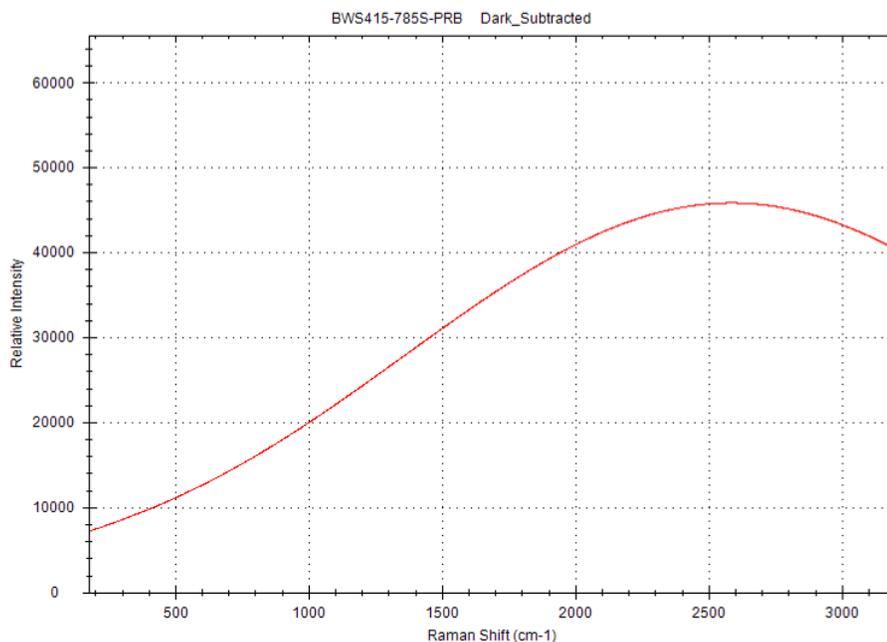
- Select **Option** → **Enable Reference Material Correction**.

- Check the box for **Enable Reference Material Correction**.

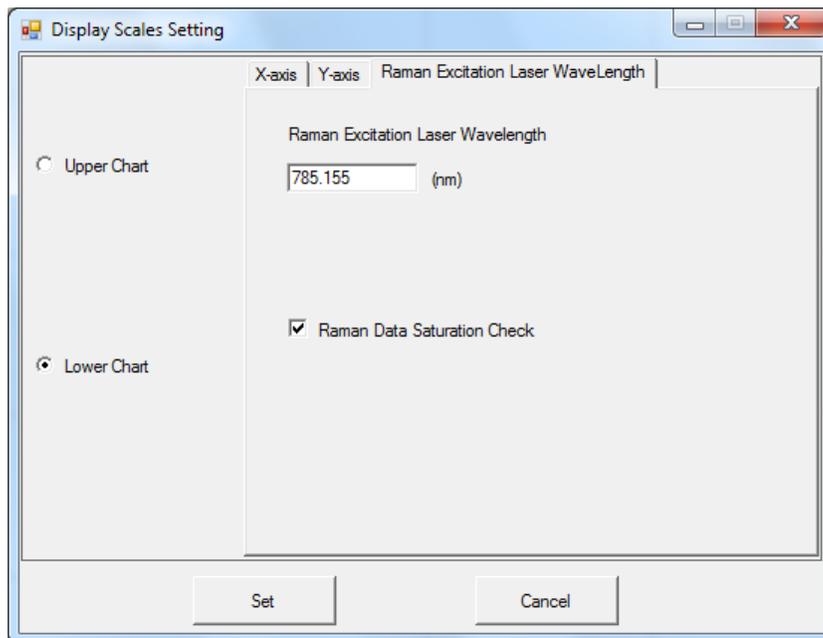
- Click  and locate the “Reference Material correction ratio2.txt” file, then click **Set**.

24.9 Relative Intensity Correction Plug-in

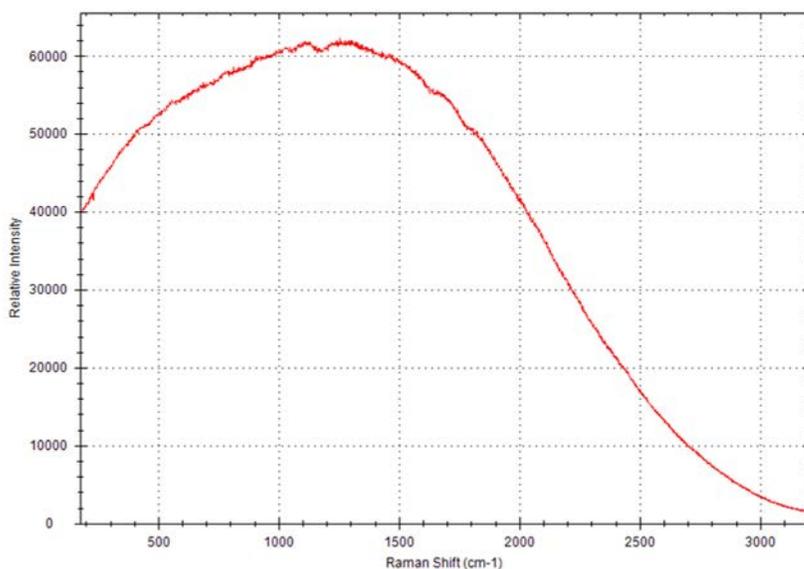
- Relative intensity correction is specific for Raman spectrometer users. Its purpose is to correct unique relative spectral responses against a traceable standard for individual spectrometers. The corrected spectral response of a Raman spectrometer makes meaningful comparisons between data obtained 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 when a 532nm excitation laser source is used and SRM2244 when a 1064nm excitation laser source is used.
- Location: Menu Bar → Tools
- **Apply Relative Intensity Correction**
 - To activate the relative intensity correction feature for data acquisition, a probe needs to be created in Hardware Setup > Probe Setup, then enable Relative Intensity Correction in Experiment Setup. See 23.3 and 15.7
 - To change the relative intensity correction setting of saved spectra, use the Batch Re-Process function.



- **How to conduct a relative intensity correction**
- This calibration comes standard with B&W Tek's applicable portable Raman systems. For advanced users, this may be conducted at a customer site with appropriate equipment. A probe must be connected to a Raman system or a laser and a spectrometer in order to get proper results.
- Ensure that the wavelength of the excitation laser you are using is entered into the **Raman Excitation Laser Wavelength** page on the **Display Scales** (for example, 785nm). You will need to determine the laser wavelength and put in the appropriate measured value.



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



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

Standard Material: SRM 2241 R2 (Raman)

Step 1: Turn off light, take a dark scan, then turn on light, take a reference scan

Step 2: Select Coefficients of the Certified Polynomial

Certified Value Polynomial Coefficient (20 - 25 Celsius scale)

$$I_{SRM}(v) = A_0 + A_1 \cdot v + A_2 \cdot v^2 + A_3 \cdot v^3 + A_4 \cdot v^4 + A_5 \cdot v^5$$

A0	0.0971937	A3	2.16023E-10
A1	2.28325E-04	A4	-9.77171E-14
A2	-5.86762E-08	A5	1.15596E-17

Step 3: Select Reference Data Use Current Reference Data Use Current Spectrum

Step 4: Select Correction Range

Left Position: 64 cm-1

Right Position: 3201 cm-1

Step 5: Set ratio file name: Ratio3_OMD

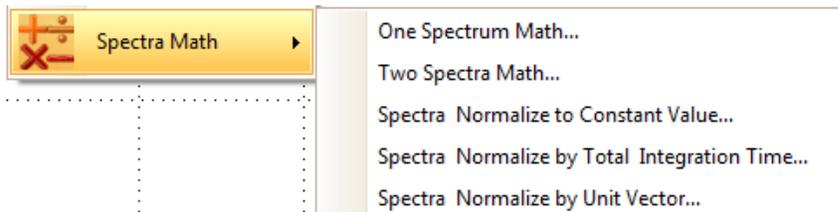
Set ratio file path: C:\BWTEK\BWSpec4\Ratio

Step 6: Create ratio file

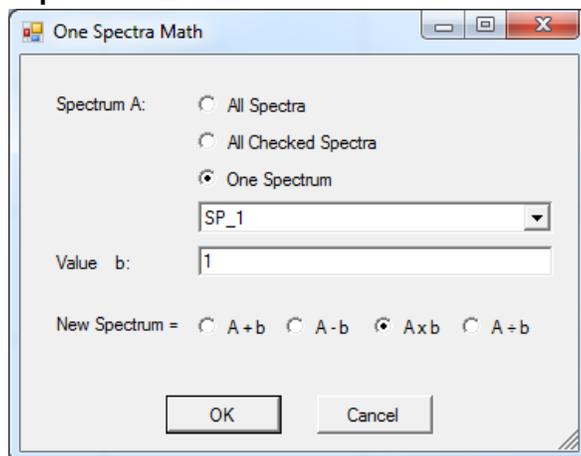
- Select the appropriate standard material (for example, SRM2241).
- Select **Use Current Reference Data**.
- Set the ratio file name and the path where the ratio file will be stored.
- Click the **Create** button. The **Relative Intensity Correction** file is created and the Ratio3 file is saved in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

24.10 Spectra Math Plug-in

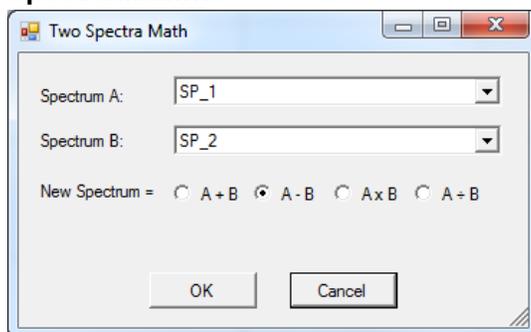
- This function provides the ability to perform math functions on a single, or multiple spectra.
- Location: Menu Bar → Tools



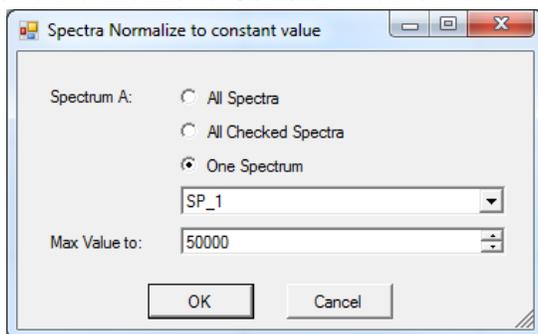
- **One Spectrum Math...**



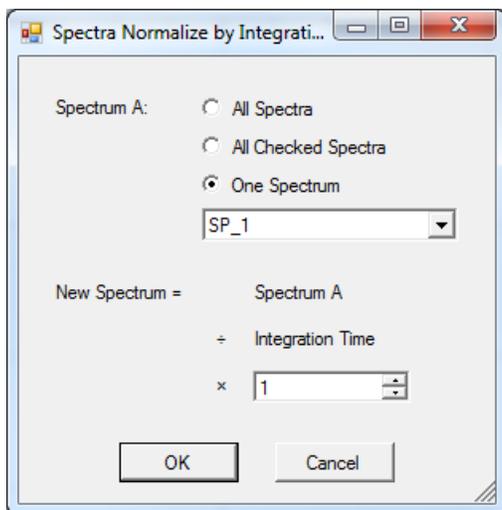
- **Two Spectra Math...**



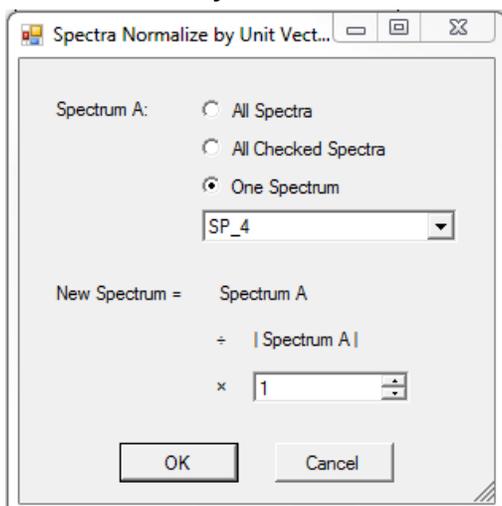
- **Spectra Normalize to Constant Value...**



- **Spectra Normalize by Total Integration Time...**



- **Spectra Normalize by Unit Vector**

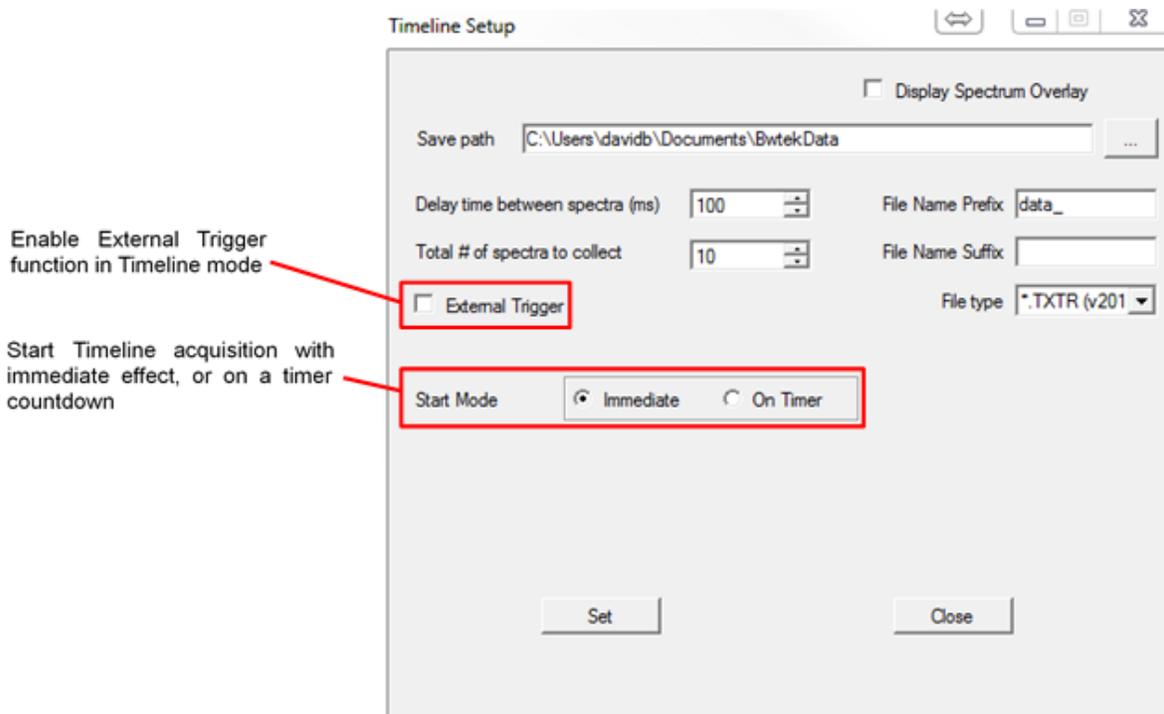


24.11 System Response Standardization

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.

24.12 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

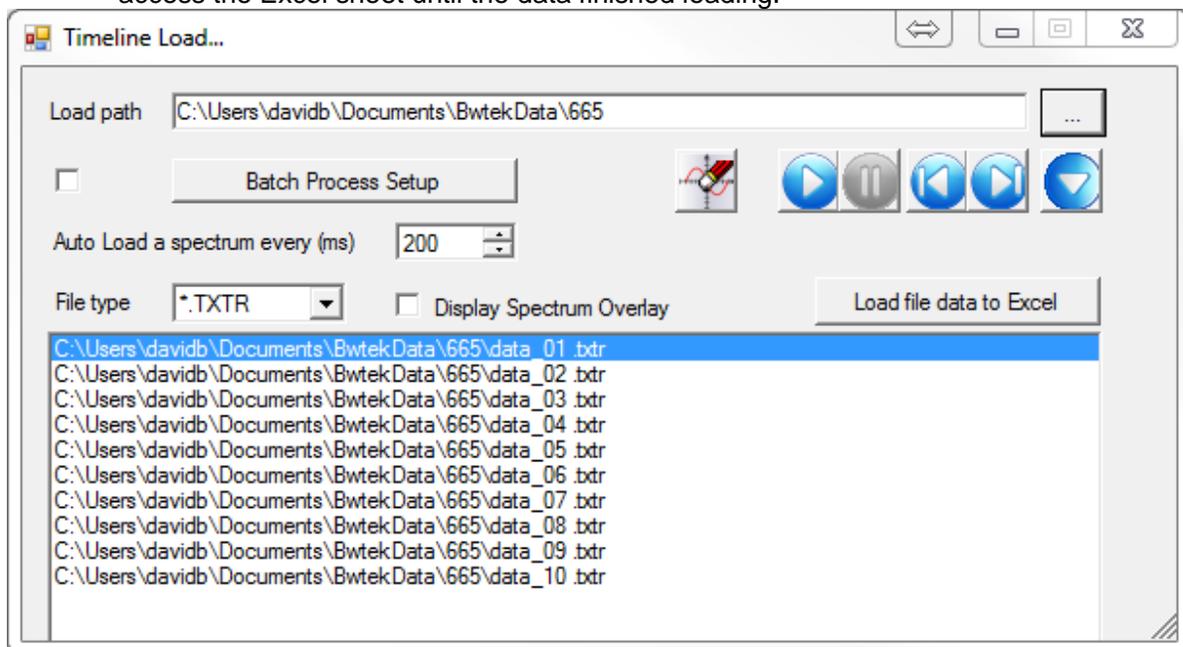


- Enter settings, including interval time (the delay time between each spectral acquisition), number of scans, file name suffix and/or file name prefix, data format for saved files and save path.
- The spectra collected will be saved in the designated path. If no specific suffix is assigned, a default 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.
- 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 and **Load file data to Excel** button to load all the data in the selected folder location into a Microsoft Excel spread sheet. Please do not try to access the Excel sheet until the data finished loading.



24.13 **Wavelength Calibration Plug-in**

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

25 COLOR MEASUREMENT

About Color Measurement

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

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

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

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

Color Measure Setup

Reference Color Setting

L: 0 a: 0 b: 0

Set Lab Value as Setting

Color Standard

Illuminant: D65

Observer: 2 degree

Wavelength for Color Calculation

Radiant Unit: mW/nm

Distance: 10 (cm)

Start WL: 350 (nm)

End WL: 750 (nm)

Interval WL: 10 (nm)

Color Calculation Source

Color Calculation Source: % T/R

Set Cancel Apply

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

A screenshot of a software interface showing a dropdown menu titled "Color Calculation Source". The menu is open, displaying two options: "% T/R" (which is currently selected) and "Irradiance".

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

A screenshot of a software interface showing a dropdown menu titled "Wavelength for Color Calculation". The menu is open, displaying several options for the Radiant Unit: "W/nm", "mW/nm" (which is currently selected), "uW/nm", "uW/cm2/nm", "uW/cm2/sr/nm", and "uW/sr/nm".

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

A screenshot of a software interface showing a form titled "Wavelength for Color Calculation". The form contains four input fields: "Radiant Unit" (set to "mW/nm"), "Distance:" (set to "10" cm), "Start WL" (set to "350" nm), "End WL" (set to "750" nm), and "Interval WL" (set to "10" nm).

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

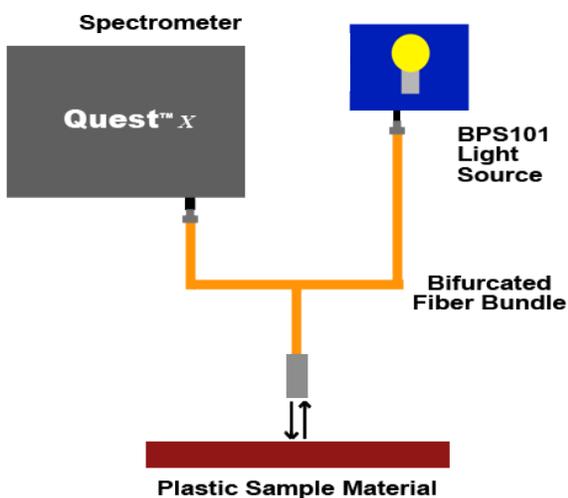
A screenshot of a software interface showing a dropdown menu titled "Color Standard". The menu is open, displaying several options for the Illuminant: "D65" (which is currently selected), "A", "B", "C", "D65", and "E".

A screenshot of a software interface showing a dropdown menu titled "Color Standard". The menu is open, displaying several options for the Observer: "D65", "2 degree" (which is currently selected), "2 degree", and "10 degree".

Reference and Dark Scan for %T/R Measurement

To perform a %T/R based color measurement, a white reflectance standard in reflectance setup and a stable light source covering the color range should be used. Light sources such as the BPS101 and BPS2.0 from B&W Tek are suitable candidates.

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



Connect the light source and the spectrometer via a fiber reflectance probe.

Turn on the light source and allow it to warm up.

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

Irradiance for Color Measurement

To perform an irradiance calibration based color measurement:

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

The screenshot shows the 'Color Measure Setup' dialog box. It is divided into several sections:

- Reference Color Setting:** Three input fields for L, a, and b, all containing the value 0.
- Color Standard:** Two dropdown menus. 'Illuminant' is set to 'D65' and 'Observer' is set to '2 degree'.
- Wavelength for Color Calculation:** A dropdown for 'Radiant Unit' set to 'mW/nm'. Below it are four input fields: 'Distance' (10 cm), 'Start WL' (400 nm), 'End WL' (700 nm), and 'Interval WL' (10 nm).
- Color Calculation Source:** A dropdown menu set to 'Irradiance'.
- Photometric Conversion:** Two radio buttons. 'Photopic' is selected, and 'Scotopic' is unselected.

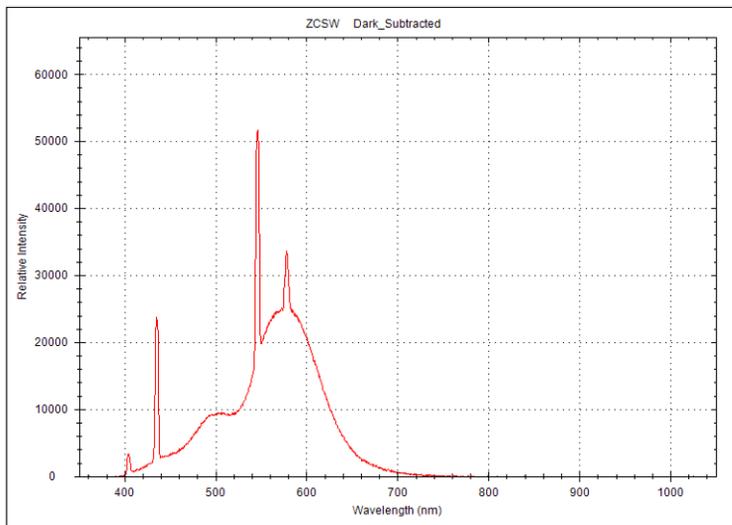
At the bottom of the dialog are three buttons: 'Set', 'Cancel', and 'Apply'.

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

Color Analysis

To acquire sample color data:

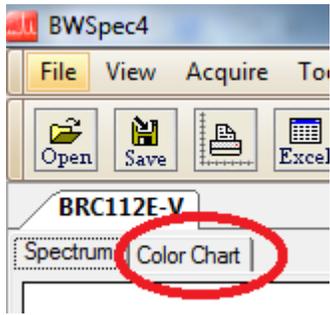
- Place the probe onto the desired sample to be measured.
- Acquire data scan on the sample material intended for color analysis.



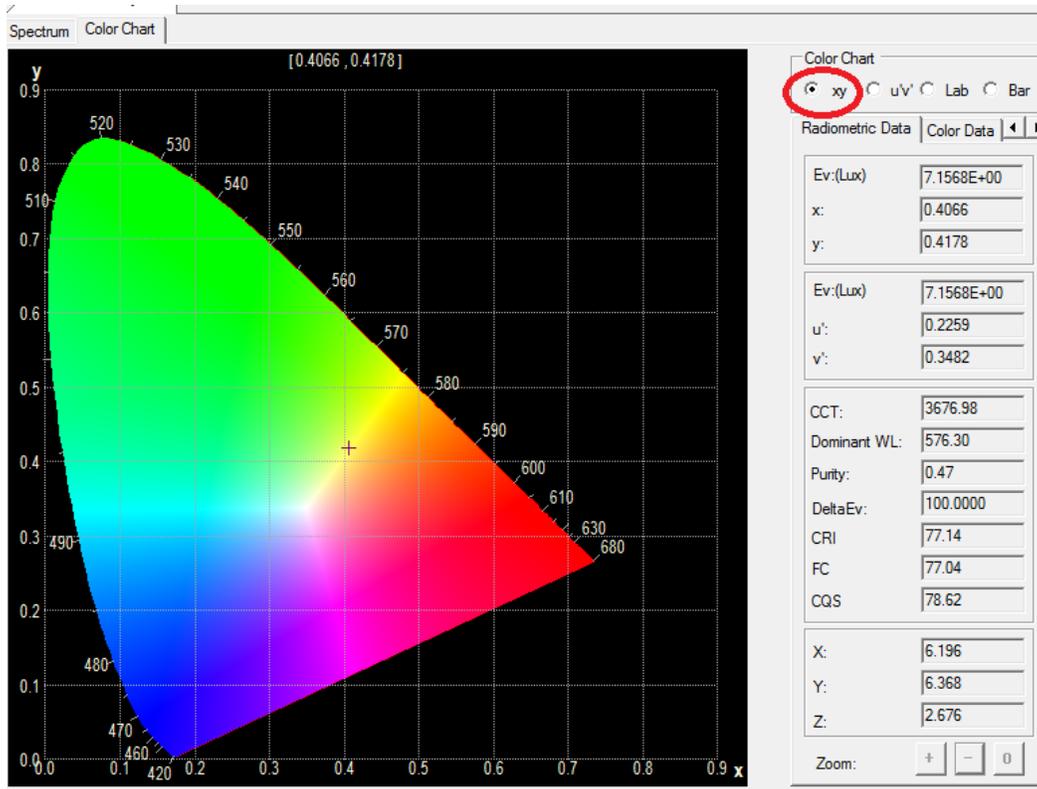
Data Display

Click the **Color Chart** tab for the chromaticity diagram and data display. (Color Chart must be enabled in the Color Measure Setup window)

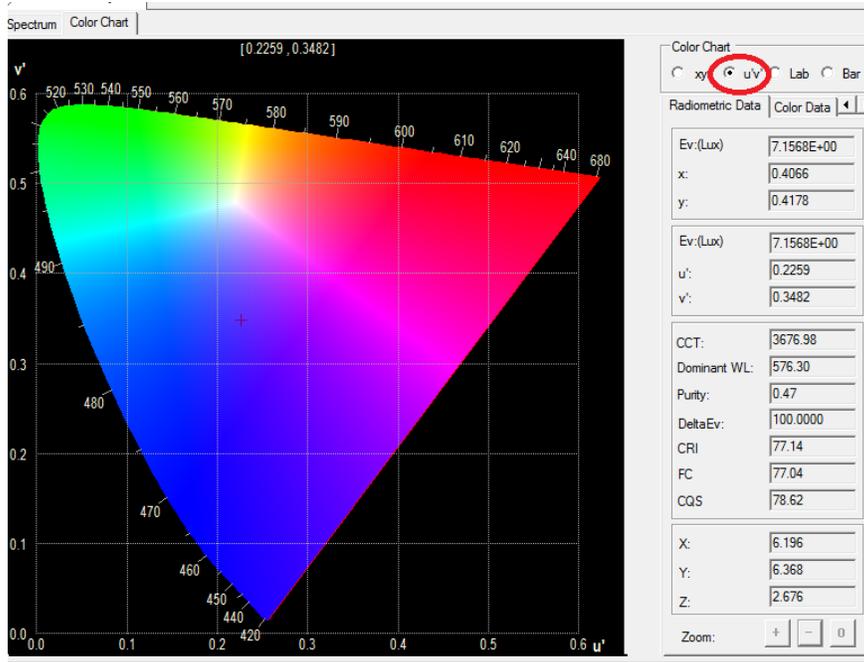
Options for four different CIE color spaces are available:



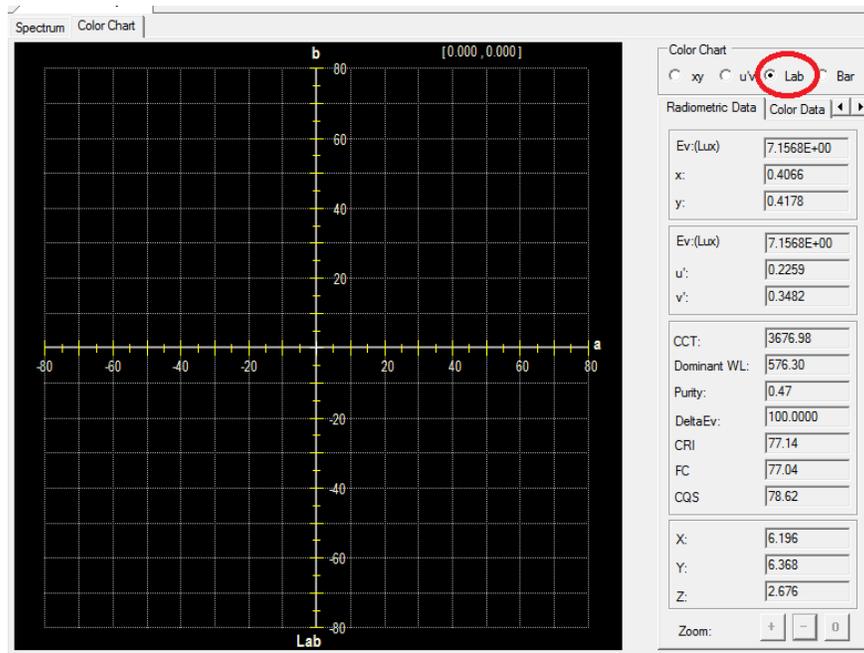
- CIE XYZ color space



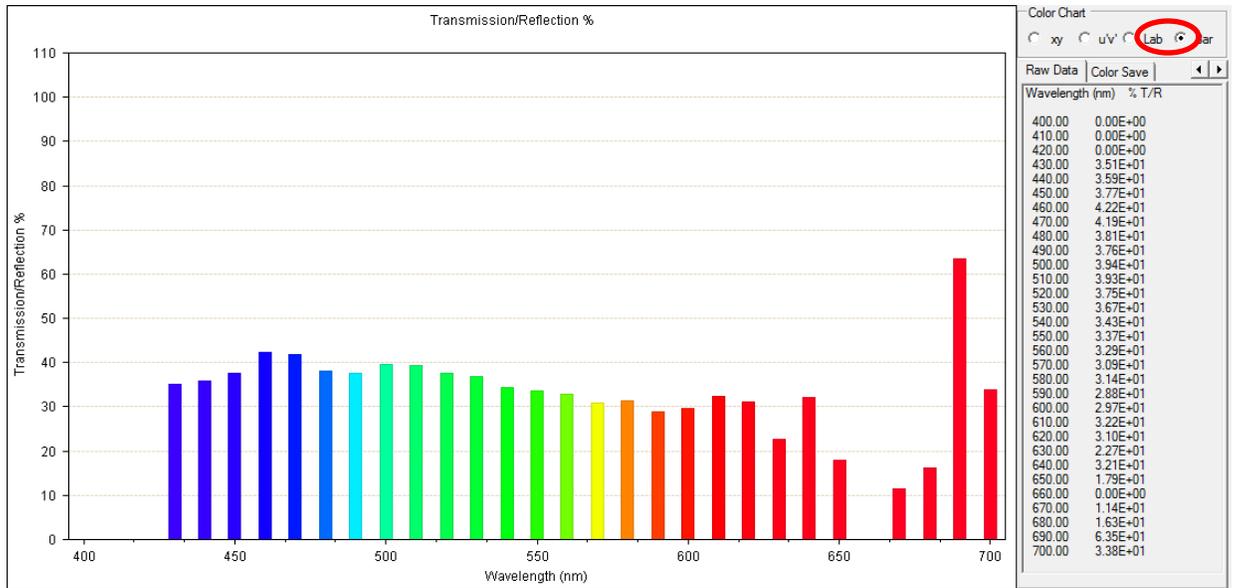
- CIELUV color space



- CIELAB color space



- Color Bar



The radiometry and chromaticity data is displayed in five categories.

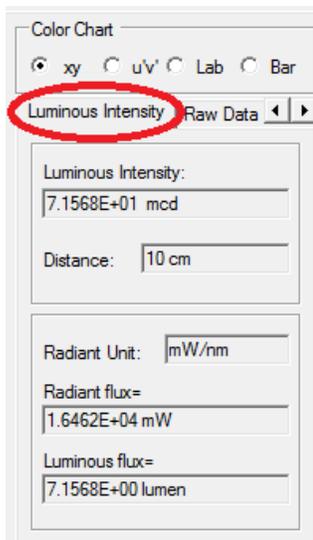
- Radiometric Data

Radiometric Data	
Ev:(Lux)	7.1568E+00
x:	0.4066
y:	0.4178
Ev:(Lux)	7.1568E+00
u':	0.2259
v':	0.3482
CCT:	3676.98
Dominant WL:	576.30
Purity:	0.47
DeltaEv:	100.0000
CRI	77.14
FC	77.04
CQS	78.62
X:	6.196
Y:	6.368
Z:	2.676

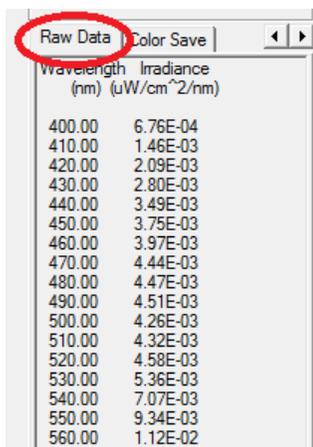
- Color Data

Color Data	
Illuminant =D65,Observer= CIE 1931 10 nm interval from 400 nm to 700 nm	
X =	6.196
Y =	6.368
Z =	2.676
x =	0.4066
y =	0.4178
z =	0.1756
u' =	0.2259
v' =	0.3482
L* =	100.000
a* =	0.000
b* =	0.000
L* =	100.000
u* =	0.000
v* =	0.000
L* =	100.000
C* =	0.000
h* =	0.000
HL* =	100.000
Ha* =	0.000
Hb* =	0.000

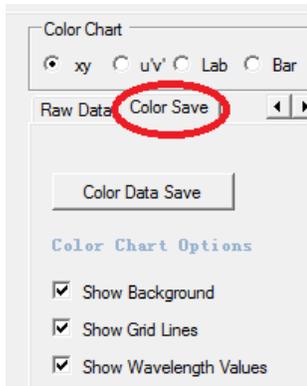
- Luminous Intensity



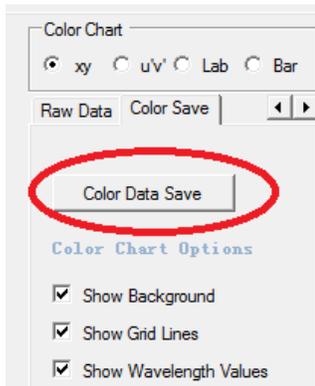
- Raw Data



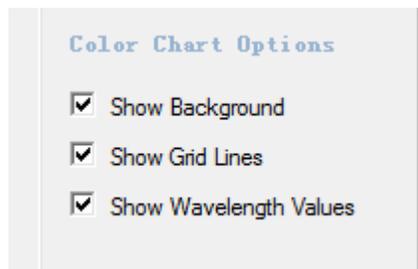
- Color Save



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



- There are three **Color Chart Options** available for color diagram settings:
 - Show Background
 - Show Grid Lines
 - Show Wavelength Values



26 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;5.6067938852322E-5		
274;7.19969136787624E-5;5.9194063207757E-5		

27 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/cm²/nm ----- lamp data unit, choice of: W/cm²/nm; mW/cm²/nm; uW/cm²/nm
S-1169 ----- designation of the standard lamp (name, serial number ...etc.)
5 ----- starting flag
250 ----- flag for starting wavelength (nm)
2500 ----- flag for ending wavelength (nm)
10 ----- increment of wavelength per data point
0.760E-05 ----- standard lamp irradiance data at wavelength = 250 nm (250+0*10)
1.788E-05 ----- standard lamp irradiance data at wavelength = 260nm (250+1*10)
3.156E-05 ----- standard lamp irradiance data at wavelength = 270nm (250+2*10)
.....
.....

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

Appendix A: Declaration of 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)
integration 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

```

```

(cosolete)
coefs_r3;3.37498265875635E-08 //The coefficients (R3) of Pixel convert to Raman shift
(cosolete)
coefs_j0;-112.640169933252 //The coefficients (J0) of Raman shift convert to Pixel
(cosolete)
coefs_j1;1.91244080985067 //The coefficients (J1) of Raman shift convert to Pixel
(cosolete)
coefs_j2;-0.000774766051834558 //The coefficients (J2) of Raman shift convert to Pixel
(cosolete)
coefs_j3;1.20204126521674E-07 //The coefficients (J3) of Raman shift convert to Pixel
(cosolete)
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 B: 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;1.0
000;1.0000;1.0000; //pixel 0 data
```

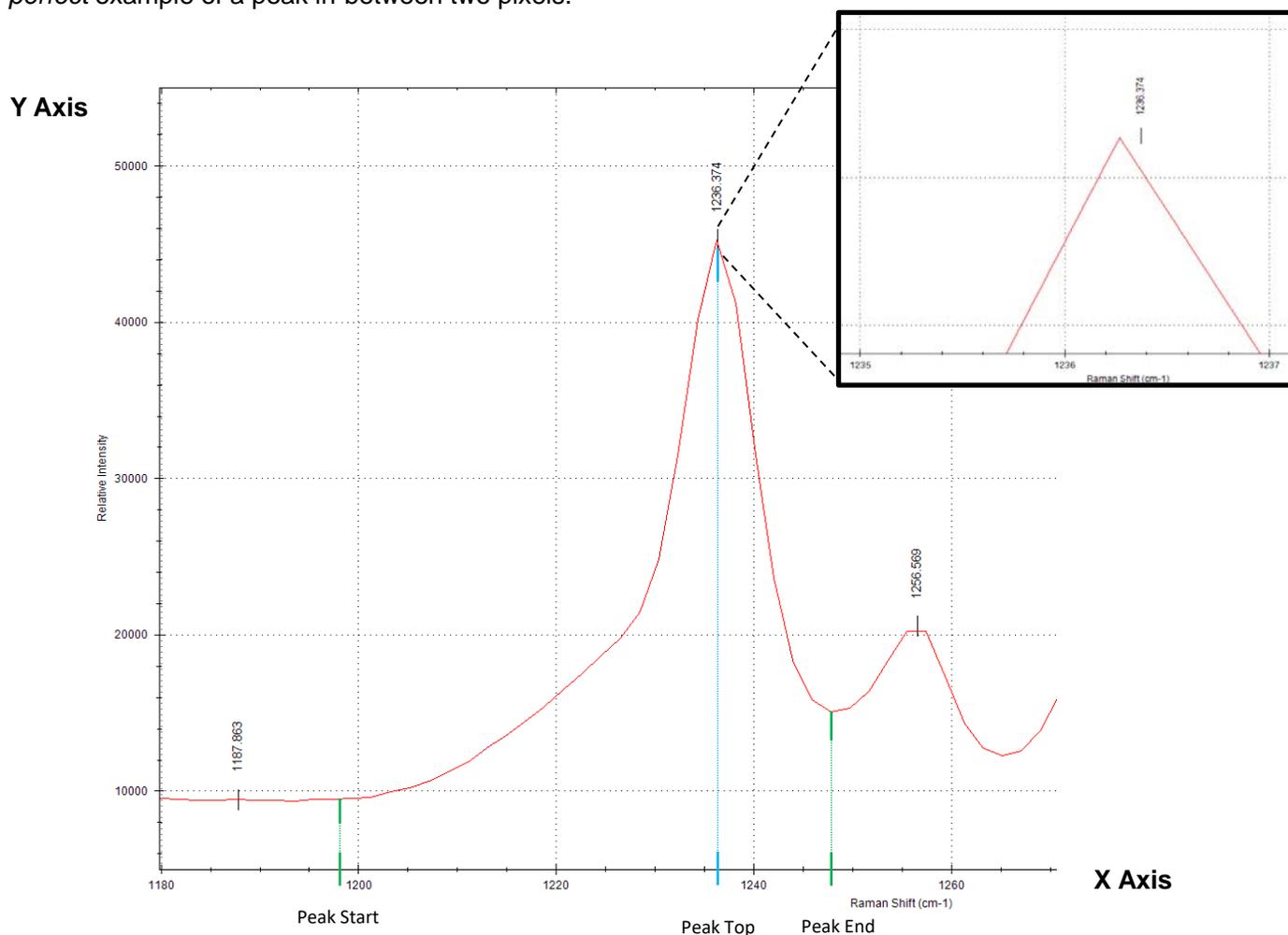
Appendix C: Peak Property Values

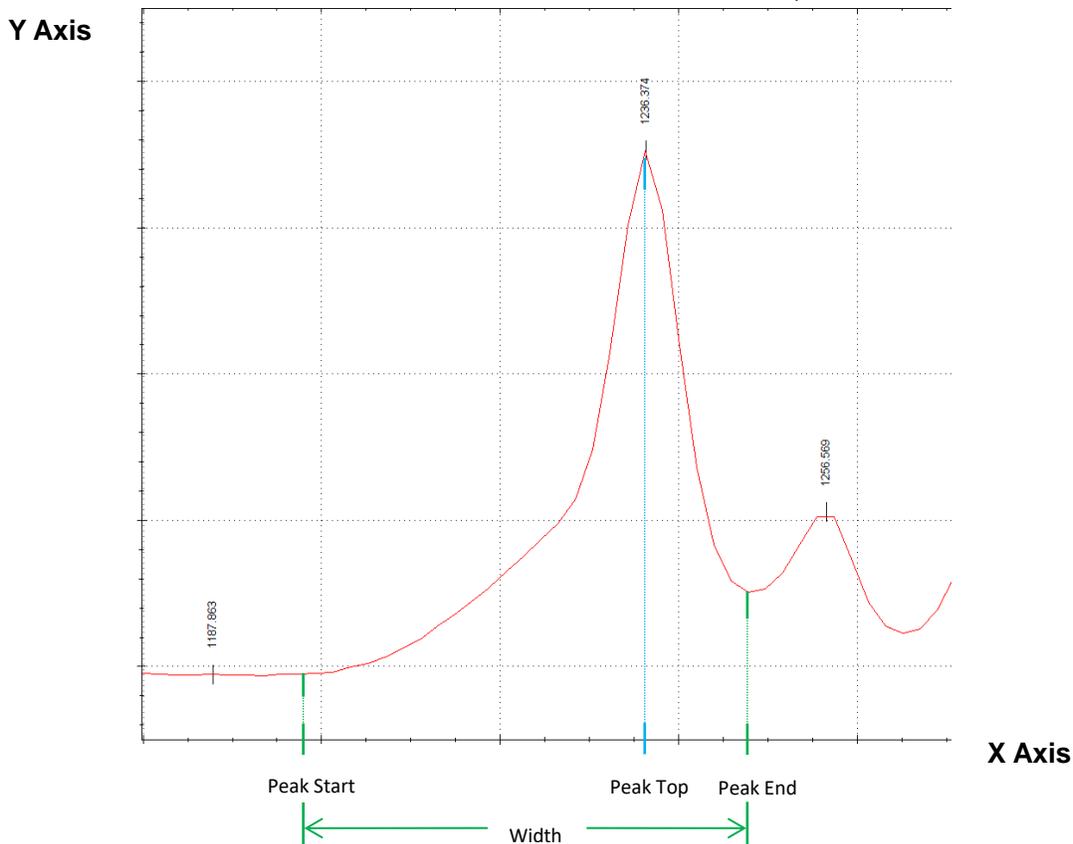
This is an overview of Peak Position and Properties, used in Peak Analysis and Peak Monitor Setup (Basic Measurement Type). Peak position is determined by curve fitting, instead of using the position of the highest pixel. This allows for a more accurate representation of the actual peak, and becomes 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).

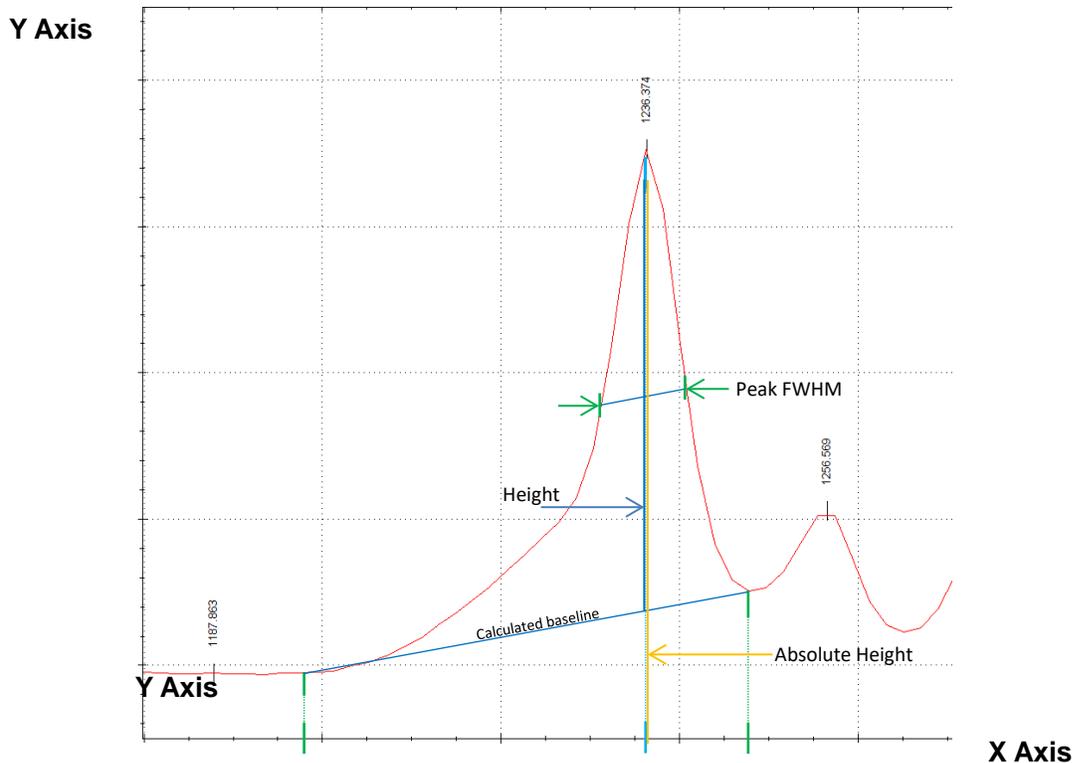
Width: Subtraction of Peak Start from Peak End.

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)



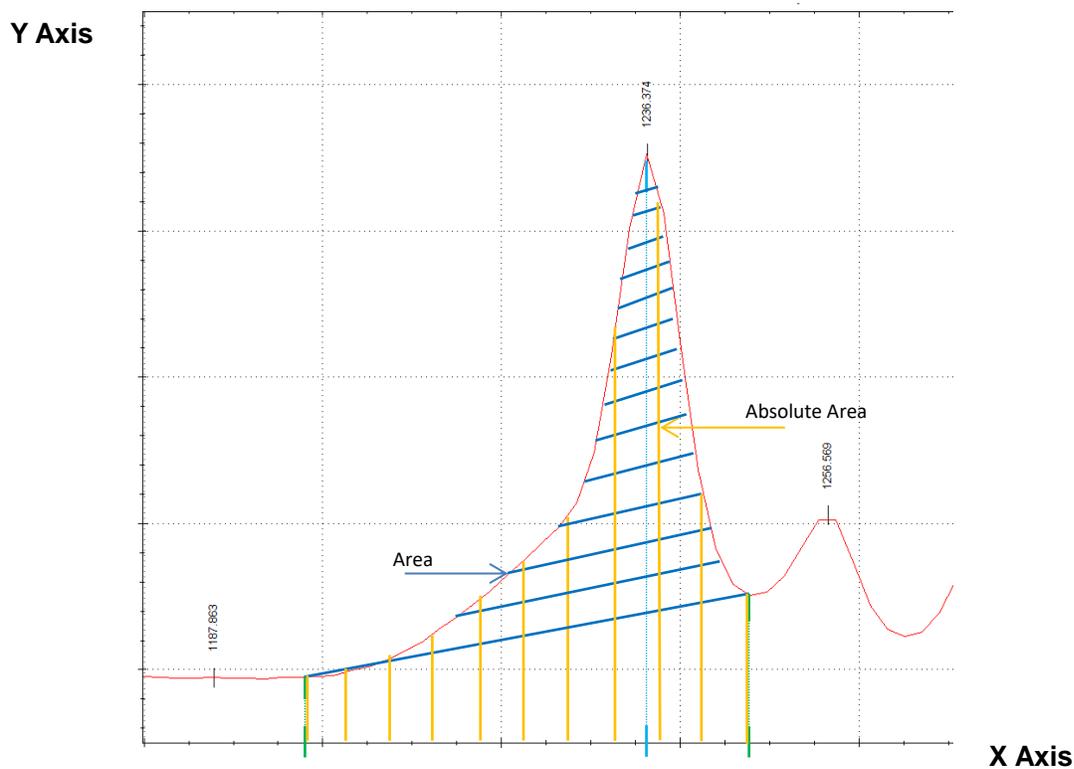
Peak FWHM: Full Width of the peak's Half Maximum. Calculated beginning from half the peak's height on each side, then the width of those half height values.

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.