

ENLIGHTEN™ SPECTROSCOPY SOFTWARE
PRODUCT MANUAL

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Document #: WP-MAN_ENLIGHTEN_1.6

Issued: October, 2019

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1 Introduction

ENLIGHTEN™ is an interactive graphical spectroscopy application designed to let users quickly and easily view and save spectra from one or more connected Wasatch Photonics spectrometers. It is intended to provide access to all of the most common spectroscopy functions via an intuitive interface that allows new users to begin taking high quality data quickly.

Caution - use of controls or adjustments or performance of procedures other than those specified herein may result in hazardous laser radiation exposure.

1.1 Manual Conventions



Advanced functions applicable to expert users or atypical (OEM, R&D) use-cases will be called-out with this icon.



Scientific and mathematical insights will be identified with this icon.



Potentially hazardous operations will be identified with this icon.

1.2 Quick Start

If the user is comfortable with Windows and familiar with spectroscopy and spectrometer control, feel free to jump right in and start using the program. Without an administrative password, nothing can be done to damage the computer or spectrometer hardware* by exploring features straight away. ENLIGHTEN™ is designed to be as intuitive and user-focused as possible, so dive in and have fun!

Please read the following guidance on eye safety before using a laser-equipped spectrometer!

1.3 Laser Eye Safety

Although a full discussion of laser eye safety is out of scope for this document, note that if using a Raman spectrometer with internal or external laser, it is of <u>extreme importance</u> to properly follow all recommended safety precautions, including:

- Know the output power level and excitation wavelengths of all lasers in operation
- Ensure that everyone within multi-path (including possible paths of light bouncing off surrounding surfaces) line-of-sight to the laser is wearing protective goggles rated for the appropriate wavelength(s) and optical density (OD) AND/OR
- Ensure that all emitted laser energy is fully captured within an enclosed, light-tight covering, whether via optic tubes, fibers, covers, housing, curtains etc.

For additional information see the following online resources:

- https://en.wikipedia.org/wiki/Laser_safety
- https://www.lia.org/store/laser-safety-standards/ansi-z136-standards





Please ensure you have received adequate training from the Laser Safety Officer for your company / facility.



2 Installation

2.1 Compatibility

2.1.1 Microsoft Windows

ENLIGHTEN™ is tested and supported on the following platforms:

- Windows 7 (32-bit and 64-bit)
- Windows 10 (32-bit and 64-bit)

Note that under Windows, ENLIGHTEN™ is compiled and runs as a 32-bit application, regardless of whether running on 32-bit or 64-bit hardware, and regardless of whether installed on a 32-bit or 64-bit version of Microsoft Windows. It will therefore be found in the "Program Files (x86)" rather than "Program Files" directory tree.

2.1.2 Linux

ENLIGHTEN™ is tested and supported on the following Linux distributions:

• Ubuntu 16.04 LTS (64-bit)

Not all features are available under Linux.

2.2 Download

The most recent released version of ENLIGHTEN™ is always available for download at the following URL:

https://wasatchphotonics.com/product-category/software/

Archive installers for older versions are provided for fault reproduction and version-locked environments, but may include bugs which have been identified and fixed in newer releases. Users are always encouraged to use the latest release version.

More advanced developmental versions are posted here (click to become an unofficial beta tester):

https://wasatchphotonics.com/binaries/apps/enlighten/

If specific software support is needed while using ENLIGHTEN™, please contact Wasatch Photonics via:

https://wasatchphotonics.com/software-support/

2.3 Application Installation (Windows)

ENLIGHTEN™ can be installed by double-clicking the 'ENLIGHTEN-Setup32-1.6.13.exe' executable installer:



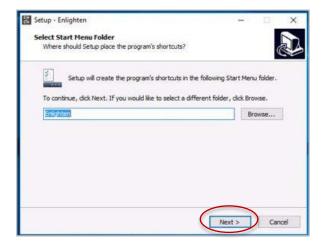
ENLIGHTEN™ installation requires administrator privileges. The user must have appropriate system access to install ENLIGHTEN™. Click 'Yes' if presented with a user account control prompt:

Wasatch Photonics ENLIGHTEN Manual 1.6.13 RAMAN edition





Choose the installation folder, or click 'Next' to accept the default.

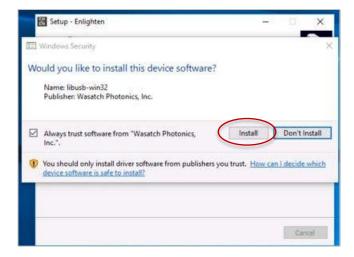


A desktop shortcut can be created, but is not required:



During the installation process, make sure to click 'Install' when presented with the driver installation portion of the installer. These drivers are required to communicate with physical hardware from Wasatch Photonics.





If the installation completes successfully, the following message (or something similar) will appear, with an ENLIGHTEN™ shortcut icon on the desktop, if the user chooses to create a desktop shortcut. Click Finish to complete the installation:



The ENLIGHTEN™ installer automatically installs the libusb-win32 drivers used to communicate with the spectrometer. If difficulties are experienced in communicating with the spectrometer, it may be worth visiting the Windows Device Manager and confirming that the libusb-win32 drivers are installed and working correctly. See section 6. Troubleshooting for additional information.

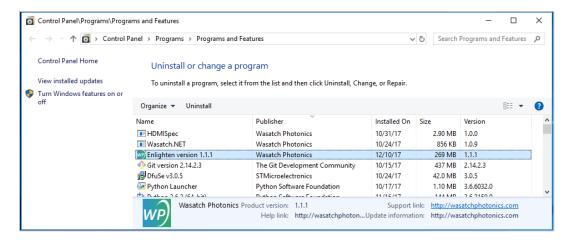
2.3.1 Updates

Users are recommended to uninstall earlier versions of ENLIGHTEN™ before installing new updates. See section **2.3.2 Uninstalling ENLIGHTEN™** for details.

2.3.2 Uninstalling ENLIGHTEN™

If ENLIGHTEN™ needs to be removed from a computer for any reason, the application may be uninstalled using the Windows Add/Remove Software control panel:





It is recommended that the current instance of ENLIGHTEN $^{\mathbf{M}}$ is uninstalled before installing a newer version of the software.

2.4 Application Installation (Linux)

ENLIGHTEN™ is distributed for Linux as a GNU tar archive containing the binary executable with a few runtime configuration files. Unarchive the tarball as follows:

```
$ tar zxvf enlighten-x.y.z-linux.tgz
$ cd enlighten
```

The only installation step is to install the udev rules necessary to allow non-root users access to USB devices with the Wasatch Photonics Vendor and Product IDs:

```
$ sudo cp udev/10-wasatch.rules /etc/udev/rules.d
```

Finally, run the ENLIGHTEN™ executable:

```
$ ./Enlighten
```

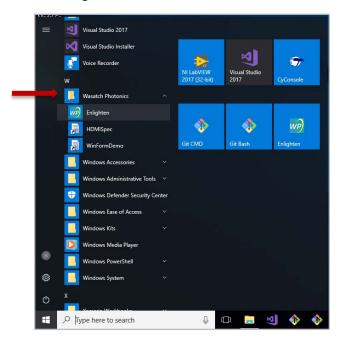
Outside of this section, the majority of this manual assumes a Windows platform, with Windows screenshots, pathnames etc. However, all described functionality should be supported under Linux with minor differences. For instance, on Linux, spectra is stored under ~/EnlightenSpectra, where the runtime configuration file enlighten.ini can also be found.



3 Starting ENLIGHTEN™

3.1 Windows Start Menu

ENLIGHTEN™ may be launched using the Windows Start Menu under the 'Wasatch Photonics' group:



3.2 Command-Line

For scripted / automated environments, ENLIGHTEN™ may also be launched from Cmd, PowerShell or bash command line shells:

For details on supported command-line arguments, see **Appendix A: Command-Line Options**.



3.3 Opening Screen

When first launching ENLIGHTEN™, if a spectrometer is already connected via USB, the software should open directly to the *Scope Capture* screen:



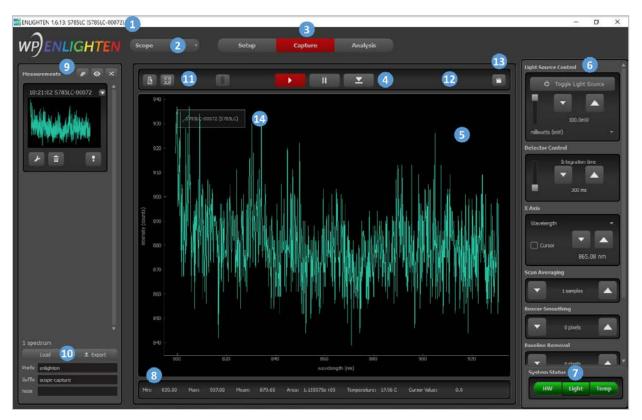
More explanation is given in section **4.1 Scope Capture** regarding the different objects and buttons above.

4 Spectrometer Operation

4.1 Scope Capture

Spectrometers are data collection instruments, and a raw "scope mode", here referred to as **Scope Capture**, is one of the most fundamental ways to visualize spectra. This mode allows the user to view and obtain "counts" directly from the spectral detector and ensure that the experimental setup is adequate prior to selecting the appropriate spectral technique and user controls. In **Scope** mode, the counts displayed are in arbitrary units.

The *Capture* mode is where most users will spend a majority of time, so it is worth learning what features and controls it offers:



Here an explanation is given in numerical order according to the labels above:

¹Window Title: A Windows title bar at the top of the ENLIGHTEN™ window that contains two fields of interest: the application version number (1.6.13 shown), and the model and serial number of the spectrometer currently connected. Both points of information will be useful when troubleshooting any issues experienced with the application.

2 Spectroscopic Techniques/Operating Modes: Shown as a pull-down menu where the user can choose the appropriate spectroscopic technique or operating mode including: *Hardware* (a special non-spectroscopic mode for device configuration), *Scope* (shown), *Raman*, *Reflectance/Transmission*, *Absorbance*, *Relative Irradiance*. The mechanics of each technique and mode are described in section 4.2 Spectroscopic Techniques and Operating Modes.



3 Functional Tab: Shown as two <u>or</u> three tabs, in ENLIGHTEN™ below the window title including: *Setup* (configuration) tab, *Capture* (data collection) tab, and sometimes *Analysis* tab depending on the selected technique and/or spectrometer. The active mode is colored <u>red</u> (*Capture* in this example).

- Play, Pause, Acquire: A trio of buttons directly above the Spectrum Chart shown as familiar mediacontrol icons (▶, ||, \blacksquare) that allow for continuous "free-running" stream (Play: ▶), freeze acquisition(Pause: ||), and save individual spectra or kick-off a Batch Data Collection (Acquire: \blacksquare). If Batch DataCollection has been enabled in Setup tab, note that the Acquire button will change from one down-pointing arrow (\blacksquare) to multiple (\blacksquare).
- **Spectrum Chart**: The *Capture* tab screen is appropriately dominated by the spectral graph, discussed in more detail in section **4.1.1.9 Chart Navigation**.
- **Ouser Controls**: The right-hand side of the screen features a scrollable palette of spectrometer and view controls, allowing you to command common spectrometer features and configure basic post-processing options. Individual controls are discussed in detail in section **4.1.1 User Controls**.
- **System Status**: Overall system health can be seen at a glance with the three status indicators at the bottom-right of the screen, which show a steady 'green' when all is well, and change to yellow or red when problems occur.
- Status Bar: Shows quick metrics about the current spectrum being displayed including minimum, maximum, mean, etc.
- Measurements Column: The left-hand side of the screen is used to track spectra that have been saved during acquisition. The Measurements Column will fill with graphical thumbnails of each spectrum as it is acquired. See section 4.2 Data Management for more information.
- Saved Data Controls: Use these controls to Load previously-captured spectra from disk, or to Export a series of saved collections as a single file for strip-chart creation and offline analysis. The user can also add to the Prefix and/or Suffix fields so that this information can be added to the filename. Adding notes to the Notes field embeds this information into the file. See section 4.3 Data Management for more information.
- Quick-Click View Toggles: In the upper-left of the chart, find buttons to lock/unlock the Y-axis (), zoom in/out to full-width chart mode (), and store/clear a quick dark () or reference () spectrum. Once a dark/reference spectrum is stored, the icon will turn red to signify it has been saved.
- **12**Status Message: When ENLIGHTEN™ wishes to display a brief status message, it will be shown here. Most messages will automatically disappear after 3 seconds.
- ©Copy to Clipboard: This feature shown above the upper right-hand corner of the Spectrum Chart (allows the user to quickly copy the currently displayed spectra (as well as the currently-selected X-axis) to the system clipboard for pasting into other applications like Excel.
- Graph Legend: Feature which identifies each individual spectrum on the Spectrum Chart. Note that box itself can be dragged elsewhere on the Spectrum Chart.

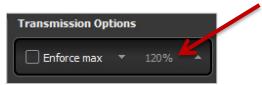


4.1.1 User Controls

The following controls are available in a vertically scrolling column along the right-hand side of all screens.

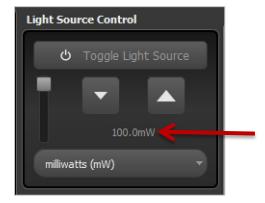
4.1.1.1 Transmission Options

Transmission Options allows the user to adjust the scale of percent transmission when in *Reflectance/Transmission* or *Absorbance* techniques. The user can set the scale to the maximum transmission allowed by the experimental setup by clicking the box next to *Enforce max*. Otherwise, the transmission can be adjusted by using either the up/down arrows or even clicking in the editable numeric field shown below with the red arrow and writing in the desired value for more precise control.



4.1.1.2 Light Source Control

This Light Source Control feature allows the user to manually turn the light source (typically an internal laser) on or off, and control the output wattage as a percentage of maximum power using either the vertical slider (upwards approaches maximum power), using the up/down arrows, or even clicking in the editable numeric field shown below with the **red** arrow and writing in the desired value for more precise control.



If the spectrometer contains a laser power calibration, this control may allow the user to switch between setting laser power as a percentage of full, and an absolute value in milliwatts.



Raman Users: If Raman users have logged-in with access to Advanced Features, they may see a 'spinner' control allowing them to specify the laser excitation wavelength in picometer precision. (Note that this does not actually <u>change</u> the emitted wavelength of your laser in real-time, but rather allows the Raman user to enter a value which is presumably generated from a high-resolution spectrometer or manufacturer's datasheet, so that $ENLIGHTEN^{TM'}$ s computed X-axis in wavenumbers will be as accurate as possible).



4.1.1.3 Detector Control

This Detector Control feature allows the user to set integration time in milliseconds (ms) using either the vertical slider (upwards increases the integration time), using the up/down arrows, or even clicking in the editable numeric field shown below with the **red** arrow and writing the desired value for more precise control.



Longer integration times will help detect extremely faint spectroscopic phenomena such as Raman Stokes scattering and fluorescence/luminescence emission, but can also increase noise and baseline by allowing more time for electrical readout noise and ambient light to accumulate. Finding the optimal integration time is dependent on the application and will most likely require preliminary experiments.

The vertical slider is deliberately capped at <u>5 seconds</u>, providing a typical range for most applications. If an integration time greater than 5 seconds is desired, the value must be selected using either the buttons or manually editing the field described above.



Note that each Wasatch spectrometer contains an EEPROM-configured "maximum recommended integration time," typically in the range of 60 seconds or thereabouts. However, longer integrations may be forced by entering values up to 2²⁴ milliseconds (4.7 hours). It is likely that electrical readout noise will saturate the detector long before you reach this range, however.

The user can also enable the external trigger if the spectrometer supports that feature. Currently only ARM-based spectrometers will show this checkbox. Please visit the following link for more details concerning Spectrometer Triggering:

https://wasatchphotonics.com/software/spectrometer-triggering/

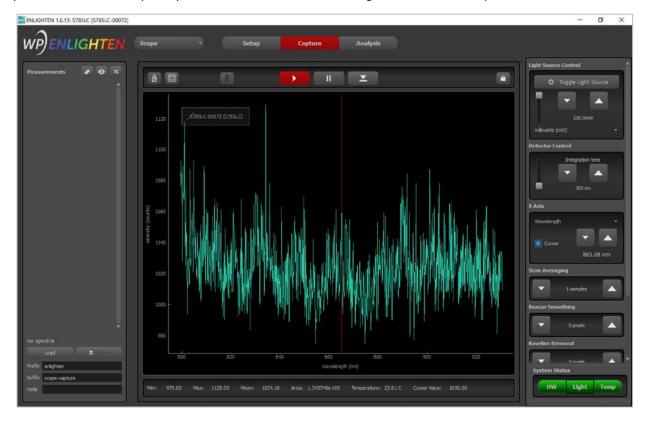
4.1.1.4 X-Axis

The X-Axis feature allows the user to select the units of the X-axis displayed on the Spectrum Chart. The pull-down menu displays three options: wavelength (nm), pixels, and wavenumber (cm⁻¹). Changing spectroscopic techniques and operating modes will reset the axis to its default state for that mode (e.g., default for *Scope, Absorbance, Reflectance/Transmission, and Relative Irradiance* is wavelength, while default for *Raman* is wavenumber). Furthermore, there is a cursor option checkbox that, when selected, displays a red vertical line on the Spectrum Chart known as the cursor. The user can set the value of the cursor by using the up/down arrows or even clicking in the editable numeric field shown below with the red arrow and writing the desired value for more precise control.





In addition, once the cursor is displayed on the Spectrum Chart, it can be selected and moved (left or right) by clicking and dragging it to the desired position. This cursor can be used to focus on a specific portion of the X-axis, perhaps, in order to monitor the changes in Y-axis at that particular variable.



4.1.1.5 Scan Averaging

One of the simplest ways to improve Signal to Noise Ratio (SNR) is by averaging over time using multiple scans. To enable this feature in ENLIGHTEN™ user can set the number of scans to average by using the up/down arrows or even clicking in the editable numeric field shown below with the **red** arrow and writing the desired value (must be a whole number greater than or equal to 1) for more precise control.







When Scan Averaging is enabled, a second text line appears on the control widget, stating "collecting X of Y" samples. This information can be used to know how soon the next fully-averaged measurement will be complete.



Note that when storing *dark* and/or *reference* spectra from the *Setup* tab, these *dark* and *reference* spectra will represent the current post-processed spectrum, with currently-applied scan averaging, boxcar, etc already applied.

4.1.1.6 Boxcar Smoothing

While Scan Averaging is the most accurate way to reduce high-frequency noise in spectral data, it comes at the cost of increased collection time. An alternative is a built-in data processing option called Boxcar Smoothing, which slides a moving average across the spectrum, averaging over wavelengths (space) instead of time. The user can set the number of pixels to average by using the up/down arrows or even clicking in the editable numeric field shown below with the red arrow and writing the desired value (must be a whole number) for more precise control. By default, smoothing is set to 0 pixels, meaning no boxcar averaging is applied.



The following example shows how a boxcar of 2 is computed across a 20-pixel spectrum. Note that the averaged (smoothed) value for pixel 6 is computed as the average of the original (raw) values of pixels 4 through 8 (5 pixels total). If a pixel is too close to the beginning or end of the spectrum to generate the specified average, original values are used unmodified.

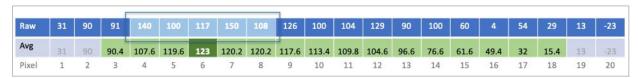


Figure 1 Computation of boxcar of 2

As seen in the following graph, the boxcar set to 2 averages-out high-frequency noise in the resulting spectrum. Please note that if raised too high, boxcar averaging will lead to a loss of optical resolution. A balance must be found between resolution and smoothing.



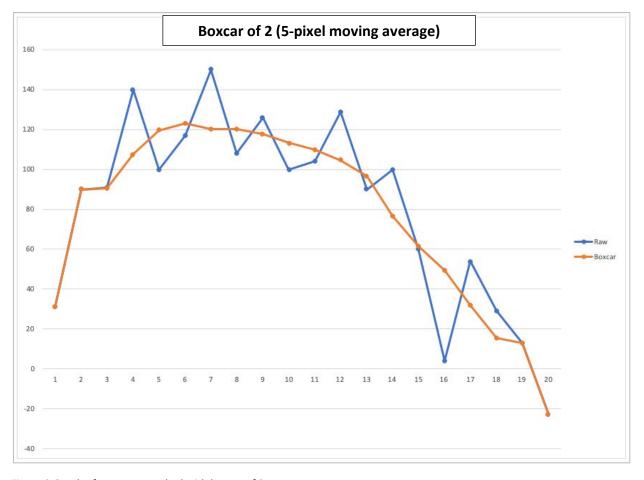


Figure 2 Graph of raw-vs-smoothed with boxcar of 2

Note that when storing *dark* and/or *reference* spectra from the *Setup* tab, these *dark* and *reference* spectra will represent the current post-processed spectrum, with currently-applied scan averaging, boxcar, etc already applied.



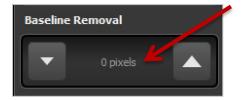
Boxcar smoothing is an example of a *convolution*, a transformation applied to an array or spectrum to yield a new array.

4.1.1.7 Baseline Removal

The Baseline Removal feature can be used to remove a majority of broadband baseline spectral features so that the detailed spectral features of the desired sample measurement remains. This feature, while not a background subtraction algorithm, is extremely useful when Raman spectra are collected for spectral matching.

This feature employs boxcar smoothing where the half-width is calculated from the number of pixels. The user can set the number of pixels for boxcar smoothing by using the up/down arrows or even clicking in the editable numeric field shown below with the **red** arrow and writing the desired value (must be a whole number) for more precise control.





The calculation for Baseline Removal can be seen as follows:

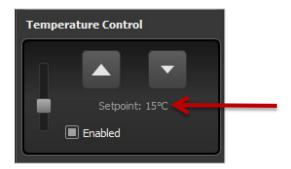
 $BaselineCorrectedSpectrum = O - C_b$

Where the resultant spectrum after Baseline Removal is *BaselineCorrectedSpectrum*, *C* is a copy of *O*, the original spectrum without baseline removal, and *b* is the half-width (number of pixels) used in the boxcar smoothing calculation applied to *C*.

4.1.1.8 Temperature Control

The Temperature Control allows the user to configure the setpoint (desired or target temperature in °C) of the detector's thermoelectric cooler (TEC). Different spectrometer models support different operating ranges with different optimal setpoints; the temperature control in ENLIGHTEN™ is automatically range-limited to the correct temperature range for any spectrometer; TEC cannot be overdriven in either direction.

In general, detectors thermoelectrically cooled to lower temperatures are capable of detecting fainter signals, as they generate less thermal noise and therefore maintain a lower, steadier baseline. The user can set the Setpoint by using the up/down arrows or even clicking in the editable numeric field shown below with the **red** arrow and writing the desired value (must be a whole number) for more precise control.





For optimal operation, it is not recommended to disable the TEC, but this capability is provided via a checkbox if you wish to compare your baseline with and without thermoelectric cooling.

4.1.1.9 Chart Navigation

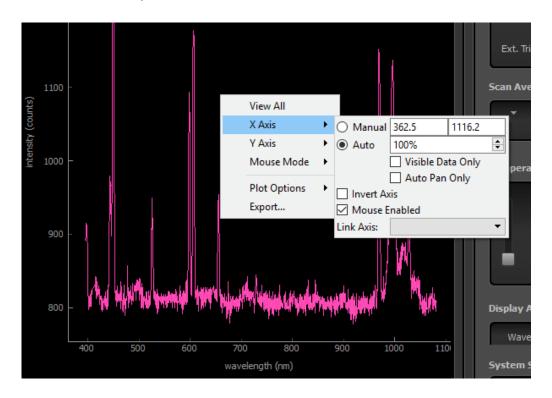
The chart display in ENLIGHTEN™ has numerous advanced features which can be accessed from a 3-button mouse or touch pad. Some of the most useful include:

 Use mouse scroll-wheel or two-finger pinch to zoom in and out (keeping the X:Y aspect ratio constant)



• Drag with left (primary) mouse button or click on left side of touch pad and drag to scroll or pan horizontally and vertically within the graph

- Drag with the right (secondary) mouse button to zoom in the X-axis, the Y-axis or both. Likewise, click with thumb (on right side of touch pad) on the desired area of the spectrum and move index finger up and down to zoom in on Y-axis or side to side to zoom in on X-axis.
- Right-click (on mouse or touch pad) on graph to open a contextual menu allowing you to finetune the X- and Y-axis, shown below:



4.1.1.10 Freezing / Unfreezing the Y-Axis

By default, the Y-axis auto-scales with each newly read spectra so this means the axis can be jumpy in high-noise environments. The lock icon atop the graph can freeze and unfreeze the Y-axis, essentially enabling and turning off the auto-scale function.

Alternately, the left (primary) mouse button or left side of the touch pad can be held down and dragged a pixel or two in any direction (vertically or horizontally). This will in turn disable the auto-scale function putting the axes into a manual mode. To re-enable the auto-scale function, right-click with the secondary mouse button or click on the right side of the touch pad to open the contextual menu, then set both X- and Y-axis back to *Auto*. Alternatively, double-click the

4.2 Spectroscopic Techniques and Operating Modes

With a Wasatch Photonics spectrometer, a user can perform a variety of spectroscopic measurements. There are some models of spectrometers that are better suited to perform a specific type of spectroscopy than others, but, here, we will describe the basic types of measurements that can be



performed. Spectroscopic measurements that can be performed with Wasatch Photonics spectrometers include:

- Fluorescence and luminescence (both are types of light emission phenomena)
- Raman (light scattering phenomena)
- Absorbance (light absorption phenomena)
- Reflectance and transmission (complimentary phenomena)
- Relative irradiance (measurement of light relative to a specific color temperature or relative to a known irradiance)

In the following sections, the user will learn which spectroscopic techniques and operating modes are necessary to perform the spectroscopic measurements described above.

4.2.1 Dark and Reference Collection Best Practices

Generally, dark measurements collected for temperature controlled detectors will not drift significantly, therefore a single dark measurement collected after the warm up of a spectrometer can last a long time, but exactly how long will vary. Reference measurements need to be frequently updated, as they need to capture the drifts in the broadband light source. If the detector is not temperature controlled, then the dark measurements will probably need to be frequently updated, since the ambient/detector temperature will change the dark measurement significantly.

4.2.2 Scope Mode

Scope mode is the simplest and most straightforward operating mode, showing the spectrum as a graph of intensity (counts). **Scope** mode is the default technique that $ENLIGHTEN^{TM}$ will open upon launching the software. The user can change the X-axis by selecting the desired unit in the X-axis User Control to pixels, wavelength or wavenumber, but by default it is set to wavelength (nm) in **Scope** mode.

Fluorescence, luminescence, and any other types of emission measurements can be performed in *Scope* mode. The user should always collect a *dark* spectrum (by clicking the button), after blocking all photons from reaching the spectrometer and prior to collecting fluorescence or luminescence emission from the sample. A dark measurement is needed to subtract any offset in the sensor signal, such that the resulting dark-corrected signal is proportional to the intensity.

4.2.3 Raman Technique

Selecting *Raman* technique in the pull-down menu changes the X-axis to wavenumbers (cm⁻¹ or otherwise known as inverse centimeters, computed as Raman shifts from the configured laser excitation wavelength), but otherwise functions very similarly to Scope mode.

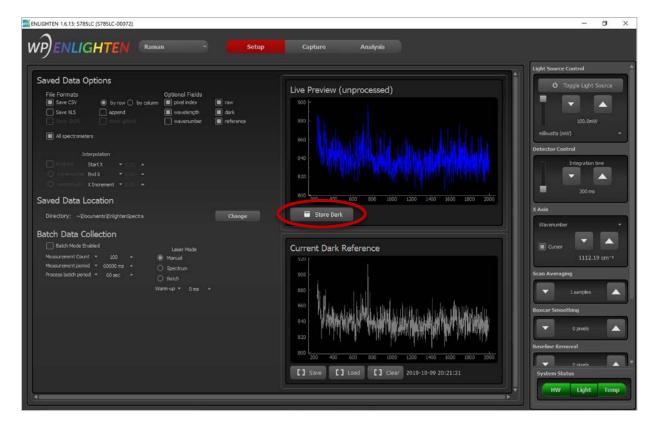
4.2.3.1 Collecting Dark Spectra for Raman Measurements

In *Raman* technique, the user must collect a *dark* spectrum. To collect a *dark* spectrum for Raman measurements the user must ensure that the excitation laser is disabled or a mechanical shutter is in place to block all light from the spectrometer. Settings such as integration time, scan averaging, boxcar, etc. must already be established because the *dark* spectrum and subsequent Raman measurement must be collected under identical experimental conditions.



After blocking all photons from reaching the detector, a *dark* must be collected so that *dark* subtraction can be carried out. *Dark* subtraction helps the always-faint Raman scattering to be detected. A dark measurement is needed to subtract any offset in the sensor signal, such that the resulting dark-corrected signal is proportional to the intensity. The user must click either the *dark* icon () in *Raman Capture* or the **Store Dark** button in *Raman Setup* to record the *dark* measurement:





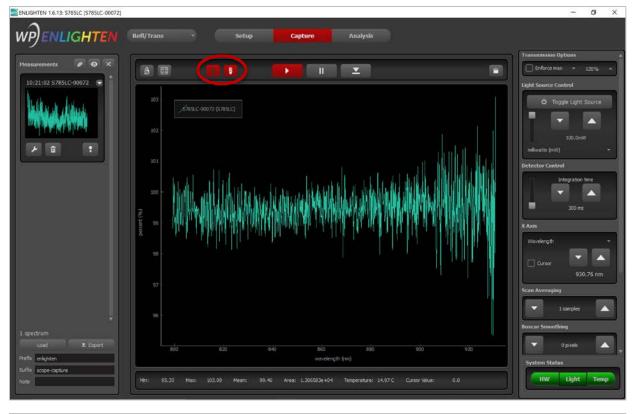
4.2.4 Reflectance and Transmission Techniques

Selecting *Reflectance/Transmission* technique in the pull-down menu changes the Y-axis to % Reflectance/Transmission, respectively. The X-axis is displayed as wavelength (nm). Transmission and reflectance are mathematically identical, although they represent physically different properties. Transmission represents the amount of light which successfully passes through a material without being absorbed, reflected, or scattered. Reflectance represents the amount of light which is reflected off a material, being neither absorbed nor transmitted.

4.2.4.1 Collecting Reference Spectra for Reflectance and Transmission Measurements

Both techniques require a *reference* spectrum, and will display a blank Spectrum Chart until a *reference* is stored. The user must click either the *reference* icon () in *Reflectance/Transmission Capture* or the **Store Reference** button in *Reflectance/Transmission Setup* to record the *reference* measurement:







For transmission measurements, the *reference* spectrum should be a direct measurement of the illuminating light source, with the transmitting sample removed from the optical path. For reflectance,

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the *reference* spectrum could be likewise a direct measurement of the illuminant, or perhaps a diffuse reflection thereof taken with a reflectance standard like Spectralon® or an appropriate synthetic resin that has equal reflectivity at all wavelengths to be measured (Delrin® or Teflon™). Similarly for Raman measurements, the *dark* spectrum used in both reflectance and transmission measurements must be collected when the illuminating source is disengaged or when a mechanical shutter is used to block all light from the spectrometer.

Resulting transmission (T) and reflectance (R) measurements are both computed using the same equation:

$$T = 100 \times \frac{sample-dark}{reference-dark}$$
 $R = 100 \times \frac{sample-dark}{reference-dark}$

Please note that *dark* spectra may change slightly over time and temperature due to detector response. It is necessary that the user make accommodations to 'dark correct' the raw spectrum using a *dark* which was taken as close in time to the spectrum as possible, so that a similar thermal environment will be in effect. Therefore, ENLIGHTEN™ will track the *dark* spectrum used with the *reference* measurement separate from the *dark* measurement used with the sample measurement, so that the 'best available' (most temporally proximate) *dark* will be used with each component spectrum.

For example, if the following measurements are collected at the specified times:

dark (d_0) at time₀ reference (r_1) at time₁ sample (s_2) at time₂ sample (s_3) at time₃ sample (s_4) at time₄ dark (d_5) at time₅ sample (s_6) at time₆

ENLIGHTEN™ will compute the transmission (or reflectance) at time₆ using the spectra collected at the following timestamps:

$$T = 100 \times \frac{s_6 - d_5}{r_1 - d_0}$$

This is because the dark, d_0 , collected at time₀ was the most-recent when the reference, r_1 , was saved at time₁, while the dark, d_5 , taken at time₅ was the most-recent when the sample was recorded at t_6 .

4.2.5 Absorbance Technique

Selecting *Absorbance* technique in the pull-down menu switches the graph Y-axis to Absorbance Units (AU), and the X-axis to wavelength (nm). Absorbance is defined as:

$$A = -\log(T)$$

This absorbance is proportional to concentration and very useful in a variety of applications. This spectroscopic technique requires both a dark and reference spectrum to be collected before the absorbance spectrum can be calculated. A dark measurement is needed to subtract any offset in the sensor signal, such that the resulting dark-corrected signal is proportional to the intensity.





4.2.5.1 Collecting Dark and Reference Spectra for Absorbance Measurements

Timing of dark and reference spectra collection can play a critical role in calculating the correct absorption spectrum. If the user collects a dark spectrum, d_1 , before collecting a reference spectrum, r, any subsequent reference measurements will be automatically dark-corrected with the most-recent dark spectrum, d_1 .

However, if the user does the above and <u>then</u> collects a <u>new</u> dark spectrum, d_2 , the resulting absorbance spectrum, A, will be computed from $(s-d_2)$ against the already dark-corrected reference spectrum, r. That is, two different dark spectra, d_1 and d_2 , will be used in the computation for final Absorbance, A, using the following equation:

$$A = -\log\left(\frac{light.transmitted}{incident.light}\right) = -\log\left(\frac{sample - dark}{reference - dark}\right) = -\log\left(\frac{s - d_2}{r - d_1}\right)$$

Where the s spectrum output by the spectrometer is the sample spectrum, d_2 is the dark spectrum taken closest in time to the collection of the sample spectrum, and d_1 is the dark spectrum taken closest in time to the reference, or r, spectrum. Please keep in mind that, when reviewing the saved data in the resulting CSV file, the Processed column will contain the final absorbance spectrum, A, from the equation listed above, the Reference column will contain the difference between the reference spectrum and d_1 , and the Dark column will contain d_2 . The spectrum known as d_1 will not be saved to the resulting CSV file.

Alternatively, if the user collects the *reference* spectrum prior to collecting the *dark* spectrum, then *r* will, naturally, <u>not</u> be dark-corrected.

$$A = -\log\left(\frac{sample - dark}{reference}\right)$$

If the *dark* spectrum, d, is collected subsequently, then the resulting absorbance spectrum, A, will be computed from the absorbance equation listed on page 26.

4.3 Data Management

ENLIGHTEN™ has several options for saving the results of measurements and experiments. Save options are configured from the *Setup* tab and triggered from the *Capture* tab.

4.3.1 Saving Spectra (*Capture* Tab)

To save a measurement to disk, simply click the **Acquire** button (▼) from the VCR-style "Play/Pause/Record" button-bar centered above the Spectrum Chart. This action adds a timestamped graphical thumbnail to the Measurement column on the left of the screen. Furthermore, each acquired measurement, by default, will be saved into a folder dated with the current date (year-month-day): This PC → Documents → EnlightenSpectra → (dated folder). For more information about how and where files are saved see section **4.3.3 Saved Data Options** (*Scope* **Tab**).



4.3.2 Thumbnail Management

With each measurement that is saved, a new timestamped thumbnail will be added to the Measurements column to the left of the Spectrum Chart. There are several options to manipulate the saved spectra through these thumbnails.



4.3.2.1 Rename the Measurement

ENLIGHTEN™ allows the user to rename a measurement while manipulating it within the software. The name of the measurement can be changed by clicking on the wrench icon () beneath the thumbnail, typing the desired name, and then pressing <Return>/<Enter> (depending on your computer) to save the new measurement name.

This will update the label shown above the thumbnail, as well as the legend in the on-screen graph (if trace is displayed), but will not change the filename on the disk of a previously saved measurement or the filename within the metadata of the file.

4.3.2.2 Delete Measurement from Disk

If the user wishes to delete the saved measurement both from within ENLIGHTEN™ and from the disk, they can do so by clicking the trash can icon () where a prompt will be shown to confirm deletion. If the user wishes to clear the current Measurements column, but leave files on disk, click the eraser icon () at the top of the bar.

4.3.2.3 View Trace

At times, it is helpful to visualize more than one spectrum on the Spectrum Chart at the same time via spectral overlay. In order to add a previously saved to the Spectrum Chart, click the ribbon icon (Several hundred spectra can be displayed at once.

4.3.2.4 Clear List

To quickly clear all thumbnails from the Measurement column (but not erase the files from disk), click the eraser icon ().



4.3.2.5 Expand/Collapse Thumbnails

The Expand/Collapse function can be applied to <u>all</u> thumbnails in the Measurement column by clicking the eyeball icon ().

4.3.2.6 Reverse Sort Order

If you want to reverse the sort order of saved spectra, so that newly saved spectra appear at the bottom rather than top of the column, click the crossing-arrows () icon at the top of the Measurement column.

4.3.2.7 Collapse

The Collapse function can be applied manually to each thumbnail by clicking the arrow pointing downward at the top right-hand side of the thumbnail graph ().

4.3.3 Saved Data Options (*Setup* Tab)

As described above, clicking **Acquire** will save spectra to disk, but choosing where the files are saved, in what format, and with what fields can be configured in **Setup** tab of any of the techniques or modes.



Here an explanation is given in numerical order according to the labels above:

¹Saved Data Options - File Formats: These check boxes allow the user to specify which file format the spectra will be saved when they are acquired. Format options include CSV, XLS, and JSON, although typically JSON is only used in specific instances. See section **4.3.3.1 Saved Data Options - File Formats** for more details.



²Saved Data Options (Details): If CSV is selected, the options by row and by column are available to allow the user to specify whether the files should be row-ordered (individual spectrum in a single row or line) or column-ordered (individual spectrum in a single column). If row-ordered is selected, it also provides an append option in which multiple spectra are added to a single file. If append is enabled, then multiple rows will be saved in a single file where each subsequent row corresponds to a unique measurement. See section **4.3.3.1 Saved Data Options - File Formats** for more details.

- 3 Saved Data Options Optional Fields: The user always has the option to select which fields are saved to resultant data files (either CSV or XLS). The options include pixel number, wavelength, wavenumber, raw, dark, and reference. See section **4.3.3.2 Saved Data Options Optional Fields** for more details.
- ⁴ Saved Data Options All Spectrometers: This feature can be used when multiple spectrometers are connected and managed through ENLIGHTENTM, typically when multiple sample setups are needed for data collection. When spectra are acquired, the software will automatically save the latest/current measurement from each spectrometer (each in a separate file, unless the append feature has been selected). See section **4.3.3.3 Saved Data Options All Spectrometers** for more details.
- Saved Data Options Interpolation: This feature allows the user to automatically interpolate spectra to a fixed / uniform X-axis when saving files. See section **4.3.3.4 Saved Data Options Interpolation** for more details.
- 6 Saved Data Location: This feature allows the user to specify where spectra are saved (defaults to Documents\EnlightenSpectra on Windows, and "~/EnlightenSpectra" on Linux).
- Datch Data Collection (Details): If the user desires to enable Batch Mode, Batch Data Collection parameters can be configured here. Options include Measurement Count, Measurement period, and Process batch period. See section 4.3.4 Batch Data Collection (Details) for more details.
- Batch Data Collection Laser Mode: Allows the user to configure how the laser functions during Batch Collections. See section **4.3.4.1 Batch Collection Laser Mode** for details.
- Live Preview (unprocessed): The Live Preview window displays a live view of the raw spectrum currently being returned by the spectrometer (i.e. no dark subtraction, boxcar smoothing or other processing applied). A dark spectrum can be collected by clicking the Store Dark button beneath this preview window. Clicking the Store Dark button triggers the same action as clicking the black light bulb (button from Capture mode. Also, a reference spectrum can be collected by clicking the Store Reference button beneath this preview window. Clicking the Store Reference button triggers the same action as clicking the white light bulb (button from Capture mode (when available). See section 4.2 Spectroscopic Techniques for more details concerning the collection of dark and reference spectra.
- ©Current Dark Reference: The Current Dark Reference window displays the most-current dark spectrum and includes any scan averaging, boxcar, or other post-processing, if applied. The date and time of collection of the dark spectrum are displayed below the window.

Current Light Reference (Reflectance/Transmission only) - not shown: The Current Light Reference window displays the most-current *reference* spectrum and includes any scan averaging, boxcar, or other post-processing, if applied (only available for techniques that require a *reference* comparison including



absorbance and reflectance/transmission). The date and time of collection of the *reference* spectrum are displayed below the window.

4.3.3.1 Saved Data Options - File Formats

Spectra can be saved in either Comma-Separated Value (CSV) or Excel (XLS) formats. Microsoft Excel can open CSV files as well. The main difference is that CSV files are more useful for dynamic programming and scripting, while the XLS files include some automated formatting and worksheet breakouts.

CSV files offer additional options over XLS files: they can be saved in either row-order or column-order format, meaning spectra can extend horizontally in rows (one measurement per line) or vertically in columns (one pixel per line).

If files are saved in XLS format, the data will automatically be saved in columns; no other option is offered. Furthermore, the files created will contain two sheets: *Summary* and *Spectrum*. The *Summary* sheet contains a timestamp and other important metadata from the time of sample collection. The *Spectrum* sheet contains the actual spectral data selected from section **4.2.3.2 Saved Data Options - Optional Fields**.

In addition, CSV files offer a special *append* option (only when *by row* option is enabled in Saved Data Optons), in which each new measurement saved is automatically appended to a single CSV file. This is a convenient means to create strip-charts of temperature and other metadata, for instance.

4.3.3.2 Saved Data Options - Optional Fields

In addition to specifying the file format of the saved files, the user can also exercise choice in what fields get written to the resultant files. Three options are included for X-axis (*pixel*, *wavelength* and *wavenumber*), and one, all, or none of the three options can be selected. However, *wavenumber* is only appropriate for Raman measurements and only available for spectrometers which have an excitation wavelength defined.

Up to three columns of signal data can be selected:

- 1. Raw Data: A relatively pure, unadulterated copy of the spectrum ENLIGHTEN™ received from the spectrometer driver. Because scan averaging and occurs in the device driver, those features are already applied to the spectrum. For this reason, it is impossible to retrieve the true raw spectrum before it is output from the device driver. However, it does not contain additional ENLIGHTEN™ processing like dark or reference subtraction or boxcar smoothing.
- Dark Data: The most-current dark spectrum that is recorded. This spectrum is then used to generate the Processed spectrum. For more details about specific calculations see section 4.2.3 Reflectance and Transmission Techniques and 4.2.4. Absorbance Technique.
- 3. **Reference Data**: The most-current *reference* spectrum that is recorded. This spectrum is then used to generate the Processed spectrum (if a *reference* spectrum is required for that technique). For more details about specific calculations see section **4.3.3 Reflectance and Transmission Techniques** and **4.3.4. Absorbance Technique**.



4.3.3.3 Saved Data Options - Processed Data Column/Row

When data is saved in the resultant file, there is a column or row of data that is always written to the file; the user cannot exclude it from being recorded. This data is saved to the Processed data column. The Processed spectrum is the spectrum displayed on-screen in *Capture* mode. This spectrum is calculated using all selected processing options, including boxcar smoothing, *dark* subtraction, background subtraction, and any per-technique processing such as applied in transmission, reflectance, absorbance or irradiance modes.

4.3.3.4 Saved Data Options - All Spectrometers

When acquiring spectra from more than one spectrometer, the serial number of all spectrometers, by default, are saved into each filename. Furthermore, the serial number is embedded into the file itself. This way, the user can confirm which data came from which spectrometer.

4.3.3.5 Saved Data Options - Interpolation

Interpolation is highly useful when comparing spectra collected from different units. The user can overlay the graphs in Microsoft Excel for comparison, and the X-axes will be consistent.

4.3.4 Batch Data Collection (Details)

Batch Data Collection allows the user to take a series of automated, unattended spectra at scheduled intervals. This is useful, for instance, if overnight spectral monitoring of a sample is desired, or if, perhaps, a strip chart of the detector's temperature over time is needed.

Batch Data Collection has four main parameters:

- 1. Batch Mode Enabled: Presents itself as a check box to enable or disable Batch Data Collection.
- 2. **Measurement Count**: This feature allows the user to set exactly how many total measurements are to be collected during Batch Data Collection. The desired *Measurement Count* can be selected by using the arrows on either side of the numeric field or by clicking directly into the editable field and entering the whole number value itself. Furthermore, up to 500 of the most recent spectra or thumbnails will be displayed in the Measurements column.
- 3. Measurement Period: Within a Batch Data Collection, this feature determines how often to collect measurements, from the start of singular spectral collection to the start of another singular spectral collection. If the user wishes to collected spectral measurements according to the set integration time, then this value should be set to 0 msec. For example, if the integration time for spectral collection is 50 milliseconds and Measurement Period is 0 milliseconds, then during Batch Data Collection an individual measurement will be collected at the completion of each integration period (essentially every 50 milliseconds). If, however, the integration time is 50 milliseconds and Measurement Period is 60000 milliseconds, or 1 minute, then during Batch Data Collection an individual measurement will be collected every 60000 milliseconds with an integration time of 50 milliseconds.
- 4. **Process Batch Period**: This feature is used to determine how often batches should be collected for continuous process mode, for example, if the spectrometer is to be left running unattended for multiple Batch Data Collections. *Process Batch Period* is the time between the start of one Batch Data Collection sequence to the start of another Batch Data Collection sequence. An



example where Process Batch Period is applicable would be as follows: a Wasatch Photonics system is turned on and left to run for 3 weeks unattended; every 5 (or 15) minutes, the system should 'wake up', collect a set of 50 measurements at a specified interval, and then 'sleep' until the next set of measurements are due to be collected.

When Batch Data Collection is enabled (box next to *Batch Mode Enabled* is checked), the **Acquire** button in *Capture* tab will change from one triangle pointing downward (\checkmark) to multiple triangles pointing downward (\checkmark). Selecting *Batch Mode Enabled* by itself does not initiate batch acquisition, the user needs to subsequently click the **Acquire** button (\checkmark) in *Capture* tab to start the acquisition.

It is very important that the user makes sure that the *Measurement period* is longer than the currently set integration time (unless the user wants to collect measurements according to the set integration time as stated above in **Measurement Period**). If Batch Data Collection is defined in which a measurement is initiated every 1 seconds, but the integration time is set to 2 seconds, it will yield the same behavior as setting *Measurement period* to 0 milliseconds (at the end of each measurement event, ENLIGHTEN™ will observe that the next measurement is already overdue and start it immediately).

As each measurement event is reached (based on *Measurement period* parameter), ENLIGHTEN^{\mathbb{M}} will act exactly as though you clicked the singular **Acquire** button ($\mathbf{\Sigma}$):

- If All Spectrometers has been checked in Saved Data Options All Spectrometers, then one
 measurement will be saved from <u>each</u> currently connected spectrometer; otherwise, only the
 foreground / selected spectrometer will be saved.
- 2. Whatever Saved Data Options are in effect at the time will determine how the measurement is saved. If both CSV and XLS options are selected, then both files types will be generated.
- 3. If it is desired that every measurement from Batch Data Collection be appended to a single file (in row-ordered format), ensure that *append* is enabled in Saved Data Options.

4.3.4.1 Laser Mode

For Raman spectrometers, it is important to decide how the laser should behave during Batch Data Collections. Three laser operational modes are supported:

- Manual: ENLIGHTEN™ makes no changes to the laser status. If the user has turned on the laser before Batch Data Collection begins, then the laser will remain on. If the laser is off prior to starting Batch Data Collection, then the laser will remain off. If the laser is toggled during Batch Data Collection, then different measurements will have different excitation states.
- 2. **Spectrum:** The laser is automatically turned on at the start of each measurement event, and turned off at the end of each measurement event.
- 3. **Batch:** The laser is automatically turned on at the beginning of Batch Data Collection, and automatically turned off at the end of Batch Data Collection. For example, if the user has determined that 1000 measurements will be collected over a three hour period, then the laser would be on/enabled for a total of three hours. Similarly, if the user wishes to analyze a sample every minute overnight (i.e. 8+ hours) then the laser would be on/enabled for a total of 8+



hours. <u>Please note this laser behavior will be cyclic if Batch Collection Process Mode is also configured</u>.

For *Spectrum* and *Batch* laser modes, if a *laser warm-up time* value is specified, that will be applied after the laser is turned on, but before the next measurement is taken. This time should be included, along with integration time, in deciding what Measurement Period you wish to configure. (Measurement Period should normally be greater than Integration Time + Laser Warm-up Time.)



Note that the *Spectrum* and *Batch* laser modes are uniquely hazardous, as they will *automatically* turn the laser on for pre-configured durations and intervals of time, including unattended/lengthy overnight data collections. It is **extremely important** that the user consider laser safety precautions before configuring unattended Raman data collections — consult with the facility Laser Safety Officer.

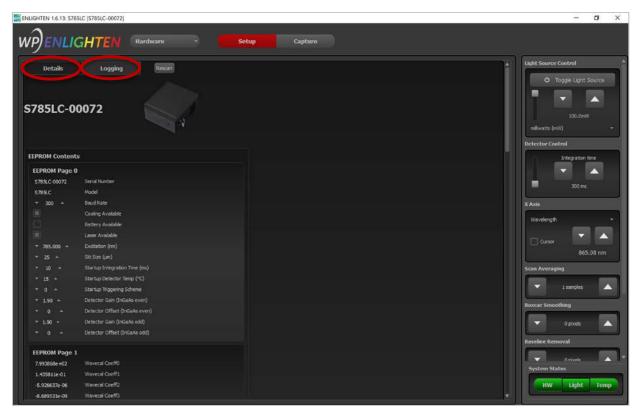


5 Hardware Configuration

Wasatch Photonics manufactures many different models of spectrometer, and, as a result, individual units within a product line will each contain unique configuration and calibration settings. Other settings, such as temperature, can vary during runtime. All of these different settings and device parameters are viewable within the ENLIGHTEN™ *Hardware* mode in the pull-down menu.

5.1 Hardware Setup

Hardware Setup has two sub-pages: Details and Logging.



5.1.1 Details

The <u>Details</u> page provides a scrollable list of hardware settings or EEPROM Contents, including excitation wavelength, wavelength calibration, TEC and gain coefficients and more. It also contains information about the spectrometer itself including serial number, slit size, whether or not there is an embedded laser, plus there is a graphic of the spectrometer connected at that time. All of this information is read-only at this time, but is useful in understanding and explaining your spectrometer's behavior and performance.

5.1.1.1 Spectrometer EEPROM

Each Wasatch Photonics spectrometer contains an EEPROM (Electrically Erasable Programmable Read-Only Memory) which stores information about the device. Parameters can be located in *Hardware Setup*, which stores configuration information about the device. Key EEPROM fields include:

- Serial number
- Excitation wavelength (internal laser models only)



- Wavelength calibration (3rd order polynomial)
- Detector temperature calibration (2nd order polynomial)
- Detector setpoint calibration (2nd order polynomial)

For a full list of EEPROM fields, see Wasatch Photonics document ENG-0034.

5.1.1.2 Gain and Offset Correction

All spectra read from the spectrometer are automatically corrected for signal gain and baseline offset based on values stored in the EEPROM These values are not user-changeable via the ENLIGHTEN™ application, although gain can be set temporarily via the .ini file (see Appendix C).

5.1.1.3 .INI Configuration

Settings stored within your spectrometer's EEPROM will be temporarily overridden while using ENLIGHTEN™ if there is a corresponding section in your .ini file which matches your spectrometer's serial number. See the Appendix C: .INI file format for additional information regarding .ini file location and contents.

5.1.2 Logging

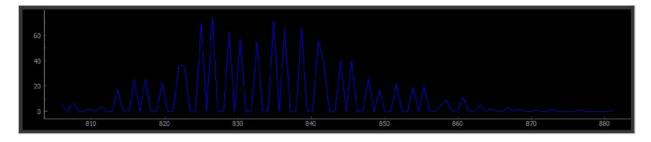
The <u>Logging</u> page shows a colorized scrolling event history of application state. The <u>Logging</u> level can be increased by ticking the "Verbose logging" checkbox. See section **6.2 Application Logging** for additional information on using the application log for troubleshooting.

5.2 Hardware Capture

Hardware Capture displays several graphs including ones for intensity histogram, live spectrum preview, laser temperature, and CCD TEC Temperature.

5.2.1 Intensity Histogram

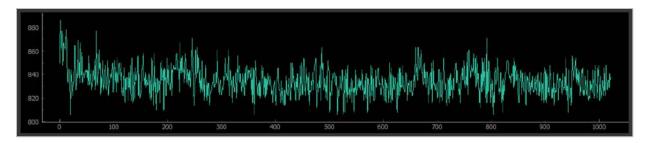
(waterfall): As an experimental feature, ENLIGHTEN™ includes a visual two-dimensional "waterfall" of recent spectra, providing a conceptual view of what monochromatic light might look like as it is diffracted across the detector. Below the waterfall is a simple intensity spectrum over the time period shown by the waterfall, and to the side is a histogram of binned intensity values by frequency. These charts are provided for hardware troubleshooting and visualization, and are not intended for spectroscopic analysis.



5.2.2 Live Spectrum View

Laser temperature is likewise graphed over time.

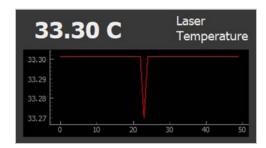




Future versions of ENLIGHTEN™ will automatically disable the laser temperature graph for non-Raman spectrometers.

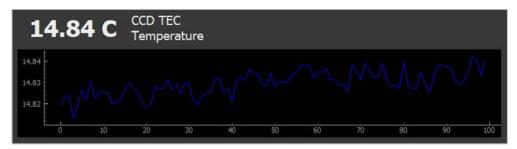
5.2.3 Laser Temperature

The historical temperature of the internal laser is graphed over time. Only applicable if the spectrometer actually has an internal laser.



5.2.4 CCD TEC Temperature

The historical temperature of the spectrometer detector is graphed over time. This allows the user to visually confirm that the setpoint and TEC are functioning as expected. The user may also generate their temperature strip-chart by using Batch Data Collection and either the CSV *append* utility or exporting a series of spectra then graphing the resulting Temperature column in Excel.



6 Troubleshooting

6.1 Common Error Conditions

Wasatch Photonics makes every effort to test ENLIGHTEN™ and our spectrometers against a variety of real-world hardware and operating environments, but the global breadth of our customer base means that there are likely some architectures and operating platforms that have not been tested. This means that the user may occasionally encounter a fault when operating our product. Should that occur, following are some suggestions to resolve the most common issues.

6.2 Application Logging

A live, colorized, scrollable version of the ENLIGHTEN^{IM} event log can be viewed within ENLIGHTEN^{IM} by navigating to *Hardware Setup* \rightarrow <u>Logging</u>.

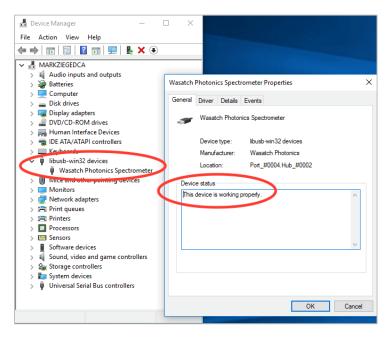
By default, the full logfile is written to the path C:\ProgramData\ENLIGHTEN™_applog.txt. Note that C:\ProgramData is a "hidden" Windows directory; to access it, the user has to actually type the directory name into the Windows Explorer and hit <Enter>...there is no way to simply "browse" to the path.

On the chance that a user encounters a problem using ENLIGHTEN™, Wasatch Photonics can best support the user by providing a resolution if the full application logfile can be sent as an email attachment. To report a problem or request a new feature, visit https://wasatchphotonics.com/software-support/.

6.2.1 Cannot Connect to Spectrometer

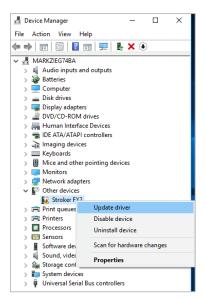
If ENLIGHTEN™ does not automatically detect and connect to your spectrometer, there may be something wrong with your driver configuration. This can be checked using the Windows Device Manager.

The current Wasatch Spectrometer <u>should be</u> listed in the Device Manager under "libusb-win32" devices, like this:





If ENLIGHTEN™ is failing to connect to your spectrometer, something like this might be seen:



If your spectrometer does <u>not</u> appear under "libusb-win32" devices as shown in the first example, please see the following URL for additional information and troubleshooting advice:

https://github.com/WasatchPhotonics/Wasatch.NET#post-install-step-1-libusb-drivers



7 Appendix A: Command-Line Options

When launching ENLIGHTEN™ from a command-line or script environment, the following command-line arguments are supported:

```
$ ./Enlighten --help
usage: Enlighten.py [-h] [-l {debug,info,warning,error,critical}]
                    [-m {setup,capture,analysis}]
                   [-t
{hardware, scope, raman, transmission, absorbance, relative_irradiance}]
                   [-o BUS_ORDER] [-g GEOMETRY] [-x]
                    [--monitor-dir MONITOR_DIR] [--overrides OVERRIDES]
                    [--run-sec RUN_SEC]
                    [--max-memory-growth MAX MEMORY GROWTH]
                    [--logfile LOGFILE]
acquire from specified device, display line graph
optional arguments:
 -h, --help
                     show this help message and exit
  -1 {debug,info,warning,error,critical}, --log-level {debug,info,warning,error,critical}
                       logging level
  -m {setup,capture,analysis}, --operation-mode {setup,capture,analysis}
                       operation mode
 -t {hardware,scope,raman,transmission,absorbance,relative_irradiance}, --technique
{hardware, scope, raman, transmission, absorbance, relative_irradiance}
                       technique
  -o BUS ORDER, --bus-order BUS ORDER
                       usb device ordinal to connect
  -g GEOMETRY, --geometry GEOMETRY
                       window geometry ('X,Y,W,H', 'fullscreen' or default
                       'maximized')
  -x, --testing
                      enable automated test support
  --monitor-dir MONITOR DIR
                       FileSpectrometer monitor directory
  --overrides OVERRIDES
                       Overrides file for raw sensor communications
  --run-sec RUN_SEC
                       Automatically exit after this many seconds (0 for
                       never)
  --max-memory-growth MAX_MEMORY_GROWTH
                       Automatically exit after this percent memory growth (0
                        for never, 100 = doubling)
  --logfile LOGFILE
                       Explicit path for the logfile
```

None of these options are required for typical usage, but this is what they are for:

--log-level Change the logging level to DEBUG, INFO, WARNING, ERROR or CRITICAL (default

is INFO). Regardless of which logging level is specified, the application will start in DEBUG mode until the first spectrometer has successfully connected (to capture detailed startup sequence), at which point the commanded or default

logging level will be applied.

The user can always switch the runtime logging level to DEBUG by clicking the

"Verbose Logging" checkbox in *Hardware Setup* → <u>Logging</u> subpage.

--operation-mode What mode the application should startup in (default is *Capture*)

--technique What technique the application should startup in (default is **Scope**)



--bus-order If multiple spectrometers are plugged-in over USB, and only one is DESIRED,

which one that should be.

This option was included to facilitate early feature testing, but may be removed

from future releases.

--geometry Whether the application should launch 'maximized' (default) or 'fullscreen' (no

menu bar) or in an 'X,Y,W,H' window (upper-left coordinate at pixel (x, y), of

width W pixels and height H pixels).

--testing Automated regression testing support

--monitor-dir In experimental/prototype configurations where ENLIGHTEN™ is not being used

to control a spectrometer via USB, but is <u>remotely</u> controlling a physical or virtual spectrometer by means of a file gateway, this specifies the watch-folder directory containing the 'spectrometer.json' file which will configure the

dataflow. (R&D only)

--overrides In experimental/prototype configurations where ENLIGHTEN™ is communicating

with a non-FID spectrometer, this parameter points to a JSON file containing various I2C byte sequences which should be sent to the spectrometer instead of

various (setting, value) pairings. (R&D only)

8 Appendix B: Keyboard Shortcuts

These keyboard shortcuts are provided to speed common operations while using ENLIGHTEN™:

- F1 change technique to *Hardware*
- F2 change technique to *Scope*
- F3 change technique to *Raman*
- F4 change technique to *Reflectance/Transmission*
- F5 change technique to *Absorbance*
- F6 change mode to **Setup**
- F7 change mode to *Capture*
- F8 use current spectrum as new dark
- F9 use current spectrum as new reference (transmission/reflection/absorbance only)
- F10 "play" (resume acquiring spectra)
- F11 "pause" (stop acquiring spectra)
- F12 "save" (capture current spectrum)

9 Appendix C: .INI file format

Your ENLIGHTEN™ installation will contain a text file named "enlighten.ini" in the following path:

C:\Users\yourname\Documents\EnlightenSpectra\enlighten.ini

(Linux systems expect the file at ~/EnlightenSpectra/enlighten.ini)

If that file is not found upon launching ENLIGHTEN™, the program will automatically create a default one

This file is used to persist application settings between runs, and also to locally override various spectrometer settings.

The following categories of application settings can be configured using the .ini file:

- Saved Data Options ("[save]")
- Batch Data Collection settings ("[batch]")
- Sound settings ("[sound]")
- Graph settings ("[graphs]")
- Logging settings ("[logging]")

In addition, the following settings can be overridden for individual spectrometers (by serial number) using the .ini file:

- integration_time_ms (int)
- boxcar_half_width (int)
- background_subtraction_half_width (int)
- detector_tec_setpoint_degC (int)
- has laser (bool)
- adc_to_degC_coeff_0-2 (float)
- degC to dac coeff 0-2 (float)
- wavelength_coeff_0-3 (float)
- detector_tec_max_degC (int)
- detector_tec_min_degC (int)
- slit_size_um (int)
- excitation_nm (float)
- ccd_gain (float)
- ccd_offset (int)
- invert x axis (bool)

This file follows a fairly straightforward syntax, and is used to selectively override individual settings from the spectrometer's EEPROM. This allows the user to customize a spectrometer's default settings, update the wavelength calibration, etc. without going through the trouble of reprogramming its EEPROM.

Each spectrometer block of the file starts with the target device serial number, followed by an arbitrary set of name-value pairs:

Wasatch Photonics ENLIGHTEN Manual 1.6.13 RAMAN edition



```
[WP-00132]
integration_time_ms = 10
wavelength_coeff_0 = 399.2413
wavelength_coeff_1 = 4.3601E-01
wavelength_coeff_2 = -7.3314E-05
wavelength_coeff_3 = 2.8049E-08
```

10 Appendix D: Saved Data Formats

ENLIGHTEN™ can save spectra in three data formats: CSV (row-ordered), CSV (column-ordered) and Excel (standard .xls).

10.1 Row-ordered CSV (Dash)

Row-ordered CSV files are saved with the following field order, which is retained for compatibility with the older Wasatch Dash spectroscopy application software:

- Line Number
- Integration Time (milliseconds)
- Timestamp
- Blank (compatibility with legacy Dash software)
- Note
- Temperature (°C)
- CCD CO (wavelength calibration)
- CCD C1
- CCD C2
- CCD C3
- CCD Offset
- CCD Gain
- Laser Wavelength (nm)
- Laser Enable
- Laser Power (%)
- Laser Temperature (°C)
- Pixel Count
- (spectral data)

The primary advantage of row-ordered CSV is that it works extremely well for appending / streaming data quickly, as it is much easier for a computer to add one line to the end of a file than to add a new column to the "right" of existing line-based data.

Therefore, this format is recommended for long-running Batch Collections taking hundreds or thousands of measurements.

10.2 Column-ordered CSV

Column-ordered CSV files are new to ENLIGHTEN™ (Dash did not support them), and as such, the file format has been adjusted. All columnar CSV files follow the convention:

- Metadata
 - o One or more lines of (name, value) pairs
- Blank
- Spectral Data
 - o A header row defining the columns for all lines to follow
 - One or more lines of spectral data (one line per pixel)



A typical column-ordered CSV might start like this:

```
ENLIGHTEN Version, 1.5.16
Measurement ID, 20190410-160240-630000-S785LC-00073
Serial Number, S785LC-00073
Label, 16:02:40 S785LC-00073
Integration Time, 10
Timestamp, 2019-04-10 16:02:40.630000
Note,
Temperature,0
CCD C0,799.3867797851562
CCD C1,0.1435811072587967
CCD C2,-5.926637186348671e-06
CCD C3,-8.689530872629803e-09
CCD Offset,500
CCD Gain, 1.9
Laser Wavelength, 785.0
Laser Enable, False
Laser Power, 100
Laser Temperature,0
Pixel Count, 1024
Pixel, Wavelength, Wavenumber, Processed
0,799.39,229.26,1276.00
1,799.53,231.51,1291.00
2,799.67,233.76,1291.00
3,799.82,236.00,1284.00
...(snip)...
```

Additional spectrum columns (after Processed) may include "Raw," "Dark" and "Reference" (see Saved File Fields).

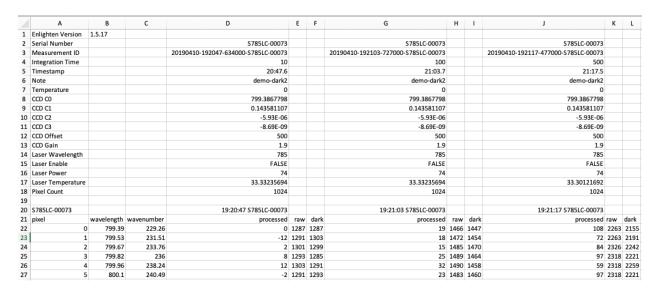
10.3 Session Exports (Column-ordered)

A special case of column-ordered CSV are "session exports," in which a number of measurements were originally saved in one format (row or column-ordered CSV, Excel, whatever), and then "exported" to a single large CSV for easy analysis in Excel or other numerical programs.

Session Exports are very similar to column-ordered CSV files, except that the (name, value) metadata is repeated atop each measurement. This is necessary, as fields within the metadata (temperature, integration time, laser enable etc) may vary from measurement to measurement, so all metadata is explicitly re-stated for measurement.

The format of a columnar Session Export might be more easily shown by example than described:

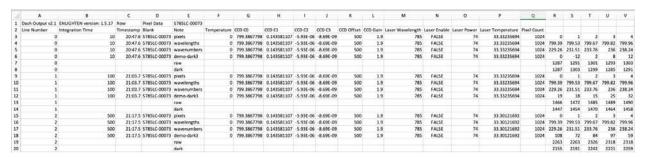




Essentially what you see there is that each spectrometer participating in the export has its x-axis columns exported ONCE (at the left of the export), and then only processed/raw/dark/reference "data" columns are populated thereafter. It is expected that users can select the proper x-axis for a given spectrometer by using the "Serial Number" row at the top of the metadata.

10.4 Session Exports (Row-ordered)

You can also export a session in row-ordered ("Dash software") format. That format (same data as above) would look something like this:



Note that "Line Number" is used to indicate "a measurement" rather than just a line, as the user selected to export 3 x-axes (pixels, wavelengths and wavenumbers) as well as 2 "component" spectra (raw and dark).

