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OMNIC for DXR Dispersive Raman

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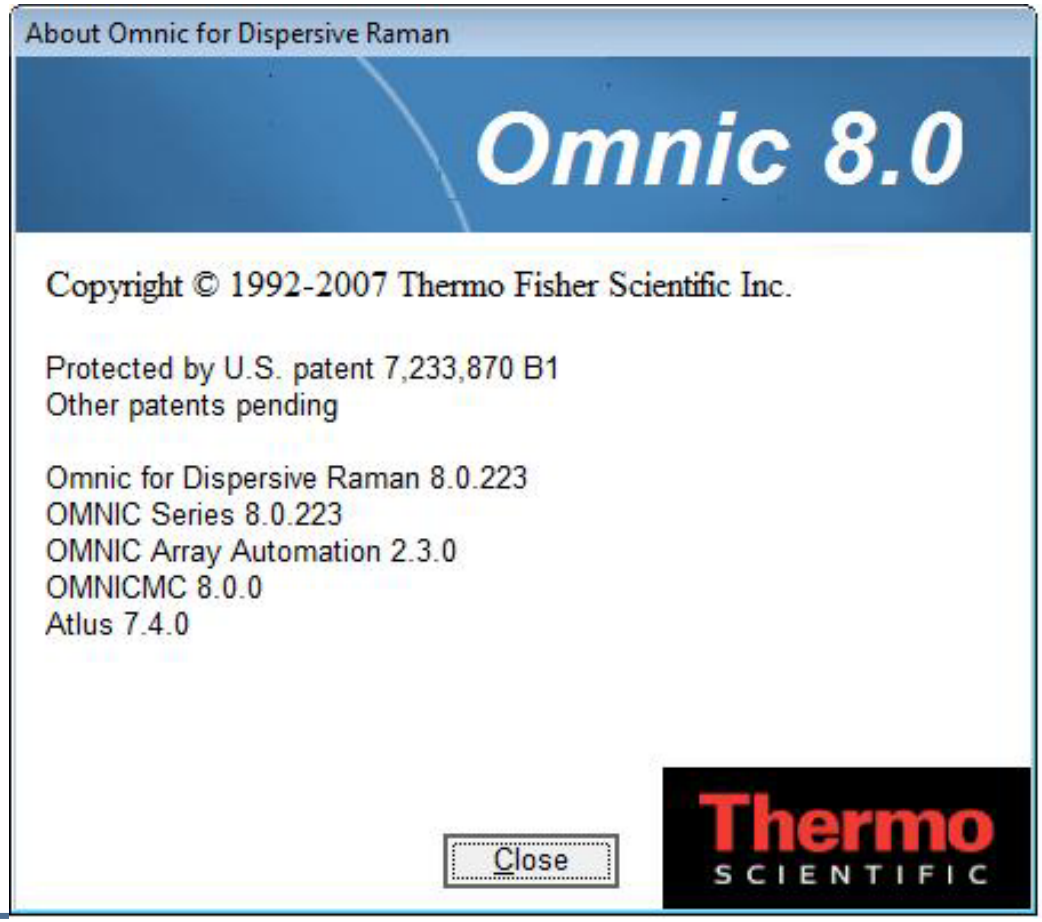
OMNIC 8.0

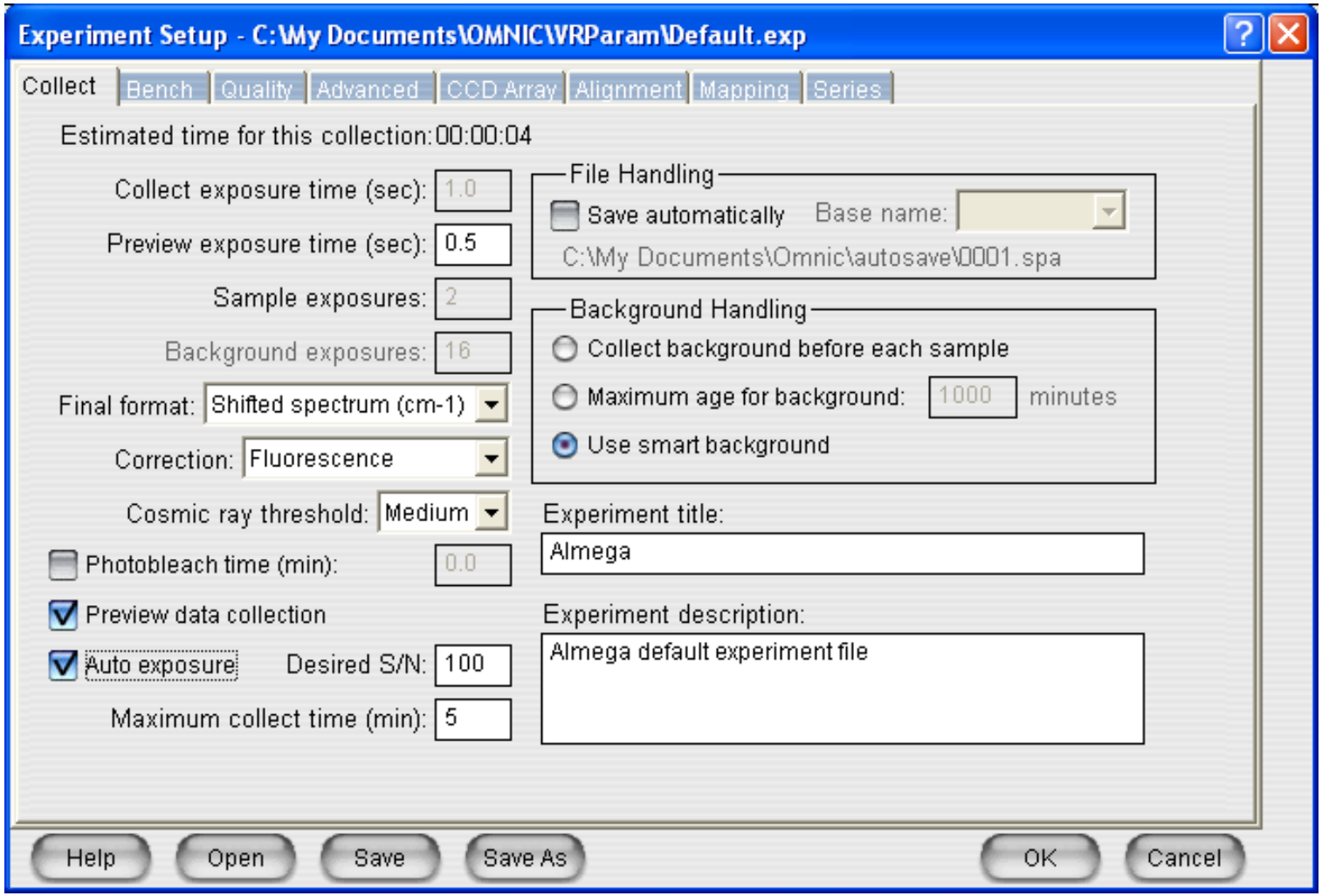
- A new version of OMNIC with new features for the DXR and Almega spectrometers is now called OMNIC for Dispersive Raman



New Features in OMNIC makes Raman Easier

You no longer need to be a Raman expert to produce high quality spectra!

Experiment Setup Collect Tab



Background Correction

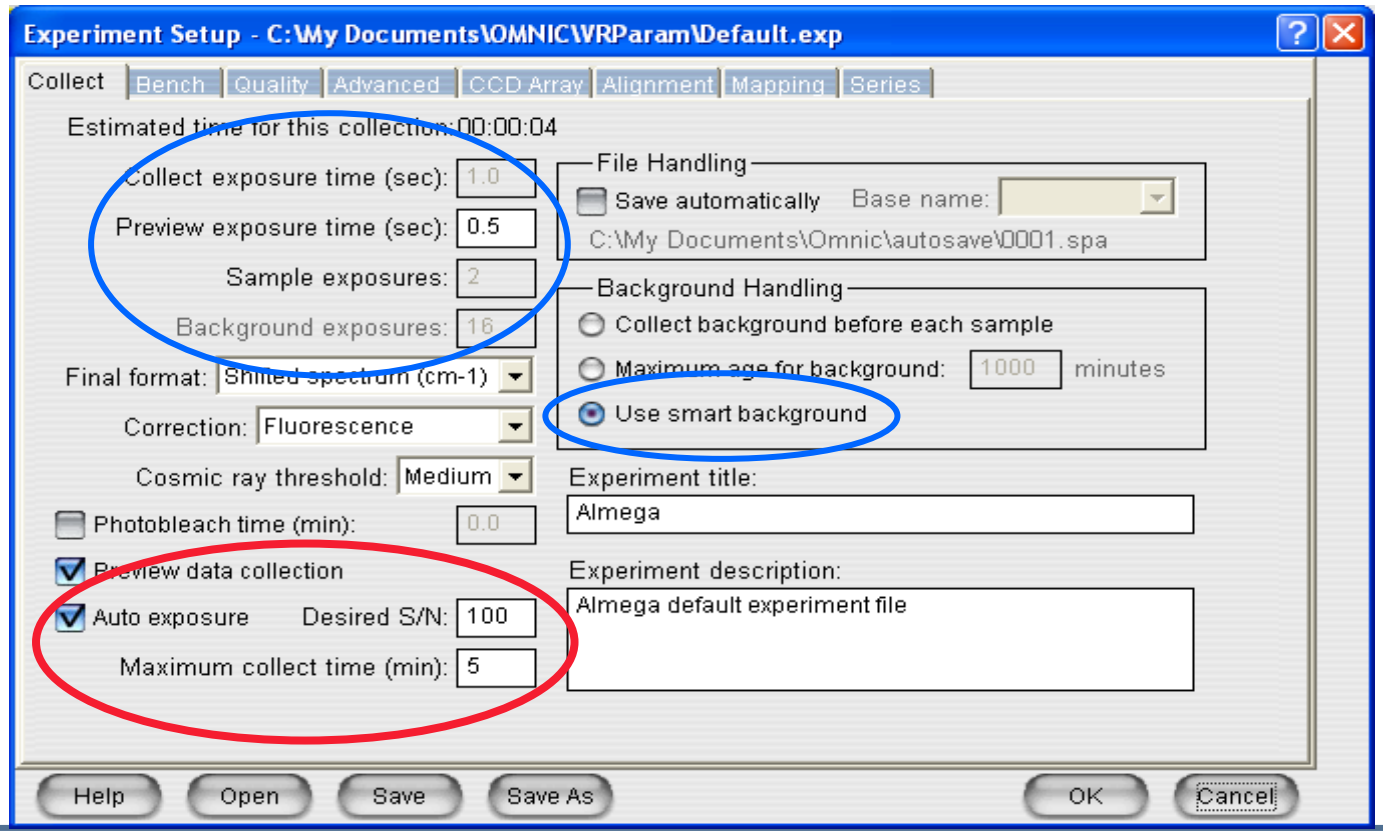
- Background correction – refers to correcting for differences in the dark state between pixels on the CCD camera due to the detector dark current (current when there is no light on the element).
- These differences result in a spectrum with subtle patterns in the baseline that have nothing to do with the sample.
- These patterns are easily corrected for by simply collecting an exposure with the shutter closed under the same conditions as the sample collection and subtracting it from the sample measurement.
- The characteristics of this detector background can change slowly over time, so it is not as simple as applying a universal correction.
- OMNIC for Dispersive Raman uses a new approach called Smart Backgrounds.

Smart Backgrounds

- Fundamentals – runs and saves backgrounds automatically when the system is not being used (OMNIC must remain open).
- Typical collection times are collected and background files stored on the computer hard drive.
- When all data for the smart background model is complete, a message to this effect is displayed. The *Use smart background* option is now enabled in the Background Handling section of the Collect tab in Experiment Setup. (A filed named bdata006250.vrb is written to the VRMCal folder containing the smart background model.)
- Benefits – saves user time when collecting sample data, can cut user time up to half potentially because the background is already collected

Autoexposure

- Allows the system to determine best collection time for a sample, makes it easier for a user, less need to be an “expert”.
- Related to Smart Background – autoexposure is only enabled when smart backgrounds are enabled.



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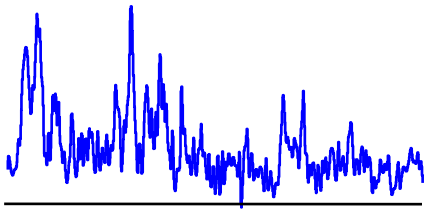
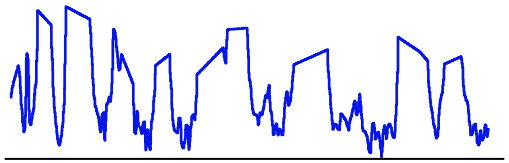
Setting Exposure Time

Under Exposed



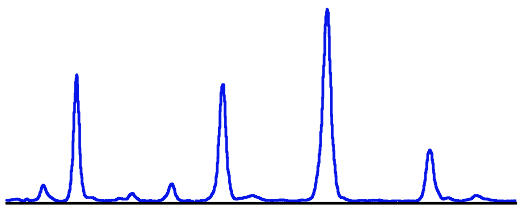
Too short - noisy spectra

Over Exposed



Too long - detector saturation

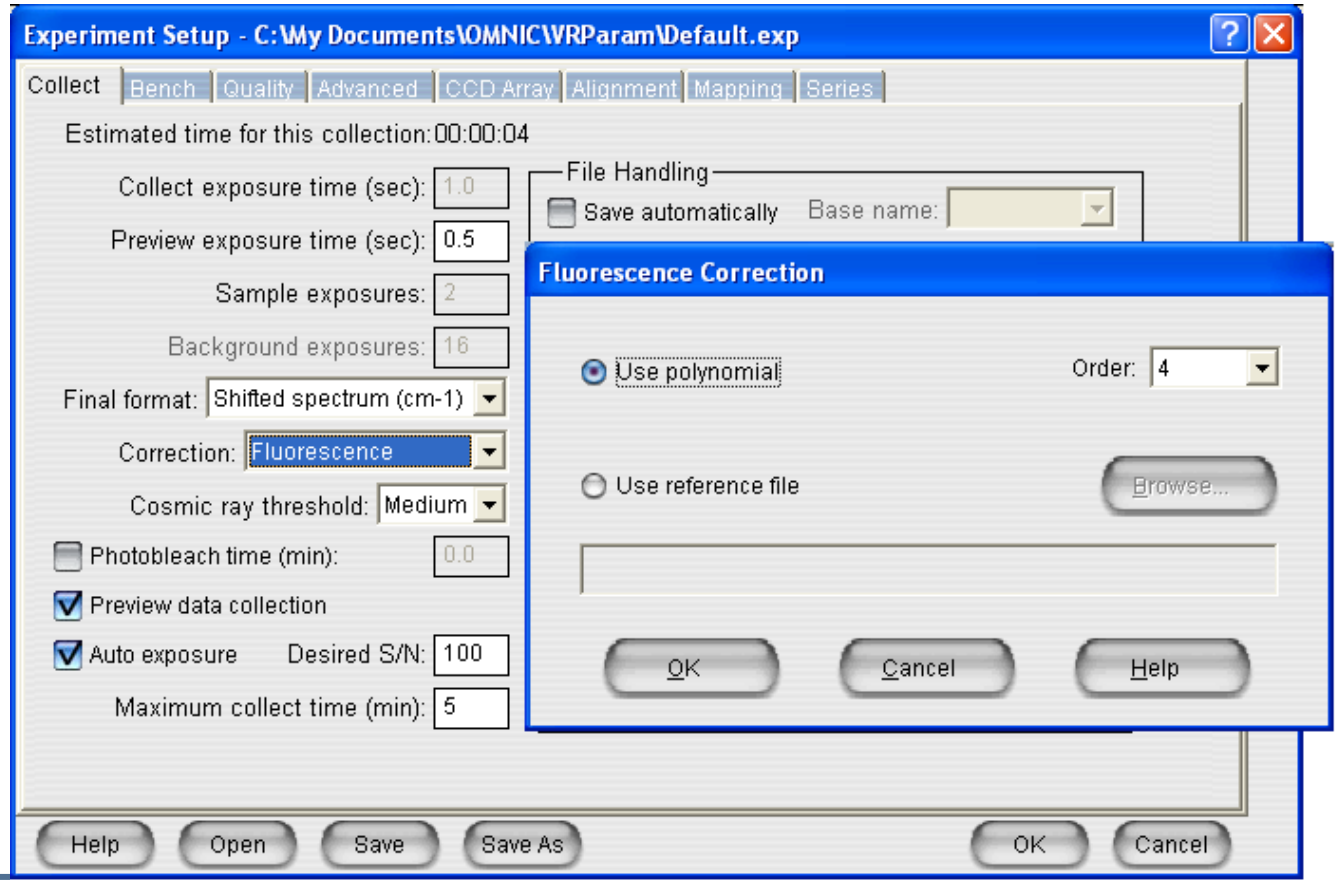
Perfect



Set correctly – high quality spectra

Autofluorescence Correction

- Some samples may fluoresce, especially with certain lasers. This correction allows the user to remove fluorescence automatically during collection.



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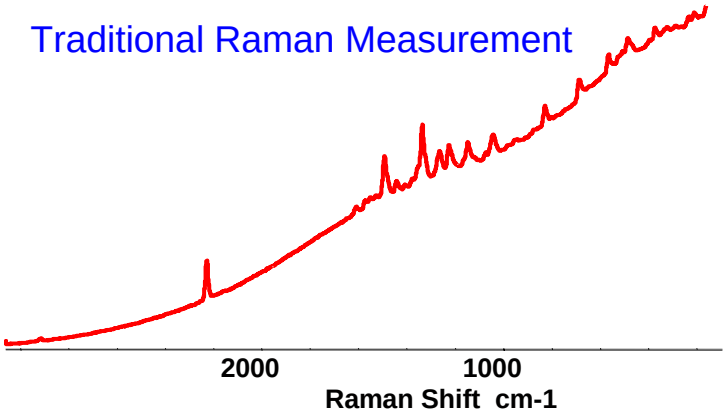
Automated Fluorescence Rejection

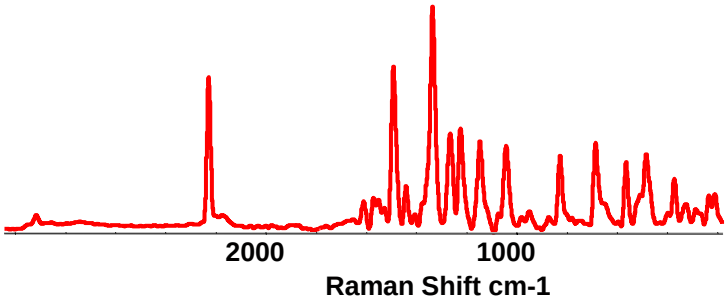
Traditional Raman Measurement



Library Search

No reasonable matches were found in this search.

Fluorescence Rejection Applied



Library Search

The best match is excellent.
The match is 5-Methyl-2-[(2-nitrophenyl) amino]-3-thiophenecarbonitrile

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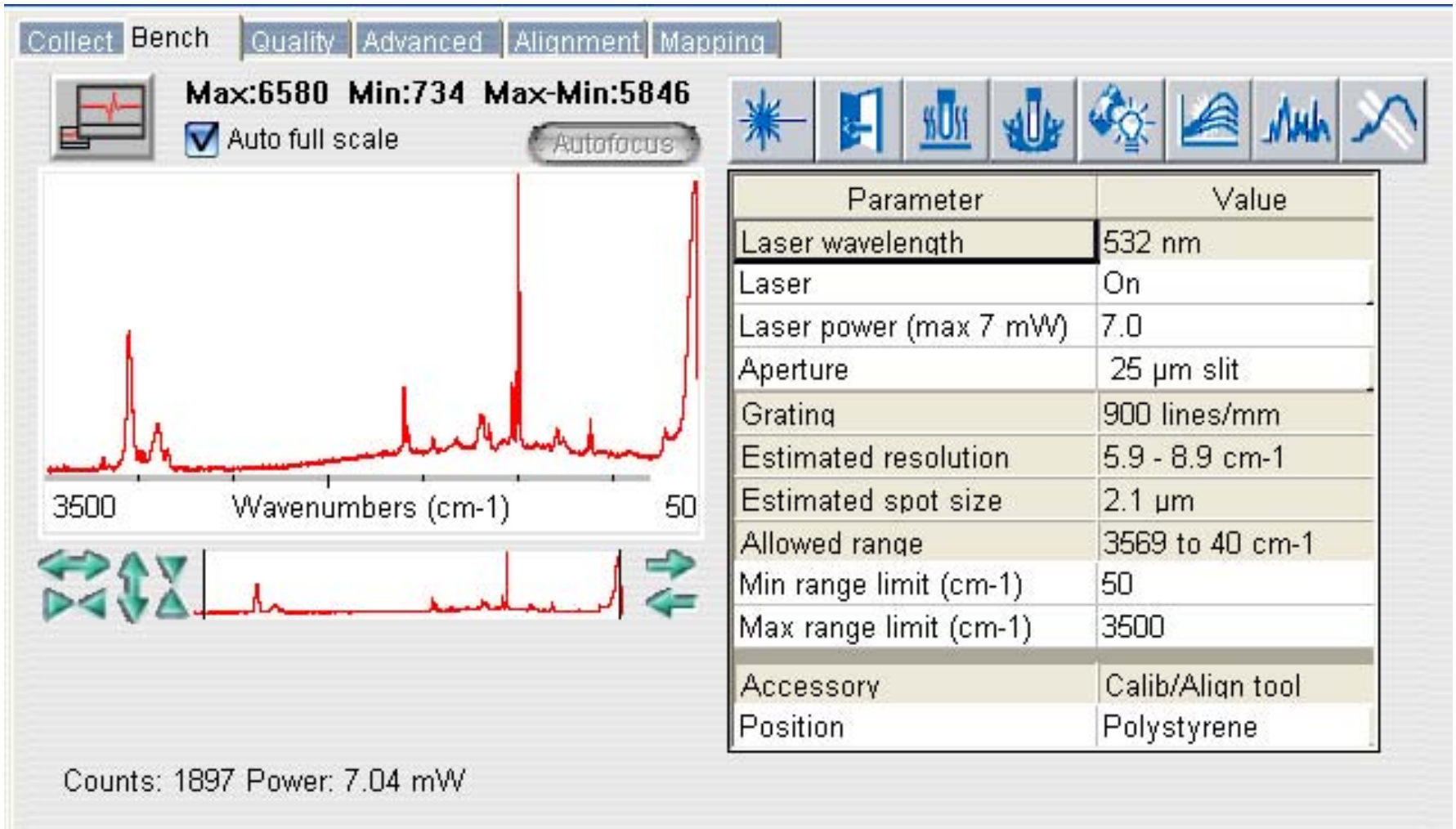
Automatic Intensity (white light) Correction

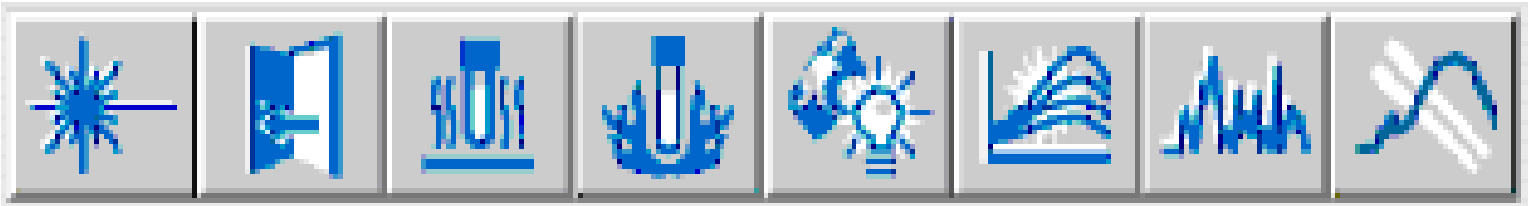
- Removes CCD wavelength response, so a spectrum collected at 532 nm can be compared to a spectrum collected at 780 nm. Makes library searching better and more reliable.
- A white light source is used during calibration (a red light is the calibration source when the 780 laser is used). The signal is collected and stored, then collected spectra are corrected after they are collected.
- DXR spectra are always corrected
  - This is done so spectra is reproducible as possible, comparable instrument to instrument and laser to laser, transferable and to remove instrument artifacts.

Bench Tab



Parameter	Value
Laser wavelength	532 nm
Laser	On
Laser power (max 7 mW)	7.0
Aperture	25 µm slit
Grating	900 lines/mm
Estimated resolution	5.9 - 8.9 cm-1
Estimated spot size	2.1 µm
Allowed range	3569 to 40 cm-1
Min range limit (cm-1)	50
Max range limit (cm-1)	3500
Accessory	Calib/Align tool
Position	Polystyrene

Status Icons in Bench Tab of Experiment Setup



Hardware icons

- Laser is off; turn on in OMNIC and turn key clockwise until vertical
- Interlock open (microscope. grating or sample compartment covers are open)

Icons linked to check marks in Quality tab of Experiment Setup

- Sample may be heating
- Sample is on fire
- CCD overflow (reduce exposure time)
- Photobleaching is occurring (non-zero baseline is decreasing)
- Weak Raman signal (increase aperture and/or exposure time)
- Sample is fluorescing (use photobleaching or purify sample)

Quality Tab

Collect | Bench | Quality | Advanced | CCD Array | Alignment | Mapping | Series

- [x] Use spectral quality checks

Collect Checks

- [x] Collect checks
  - [x] CCD overflow

Spectrum Checks

- [x] Spectrum checks
  - [x] Sample heating
  - [x] Fluorescence
  - [x] Sample burning
  - [x] Photobleaching
  - [x] Weak signal

Minimum: 15

This corresponds to the Max-Min value above the live display in the Bench tab.

Advanced Tab

Collect | Bench | Quality | Advanced | Alignment | Mapping

Data spacing: 0.964 cm-1 (2 cm-1 FT) ☑ Set spacing automatically

Camera temperature: Cooled Laser usage: 790 hours

☑ Laser saver after 300 minutes ☑ Turn laser off when OMNIC closes

Maximum calibration age: 30 days

Maximum alignment age: 30 days ☑ Recalibrate after alignment

Maximum smart background age: 180 days

Macro for Go button: Browse...

Autofocus

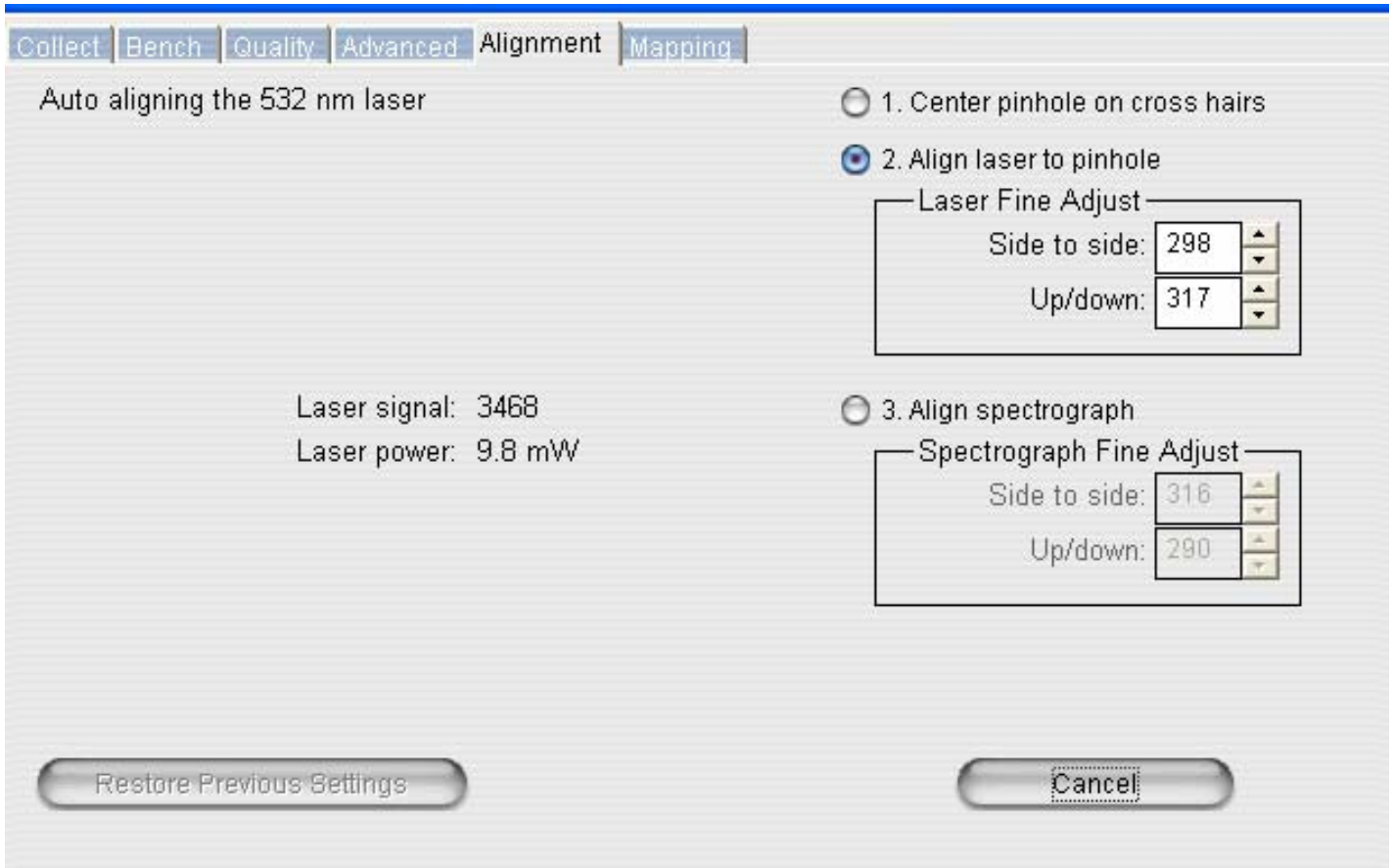
☐ Before collection ☐ Ignore fluorescence

☐ Autofocus background Browse...

☐ Prompt when collecting if laser is off

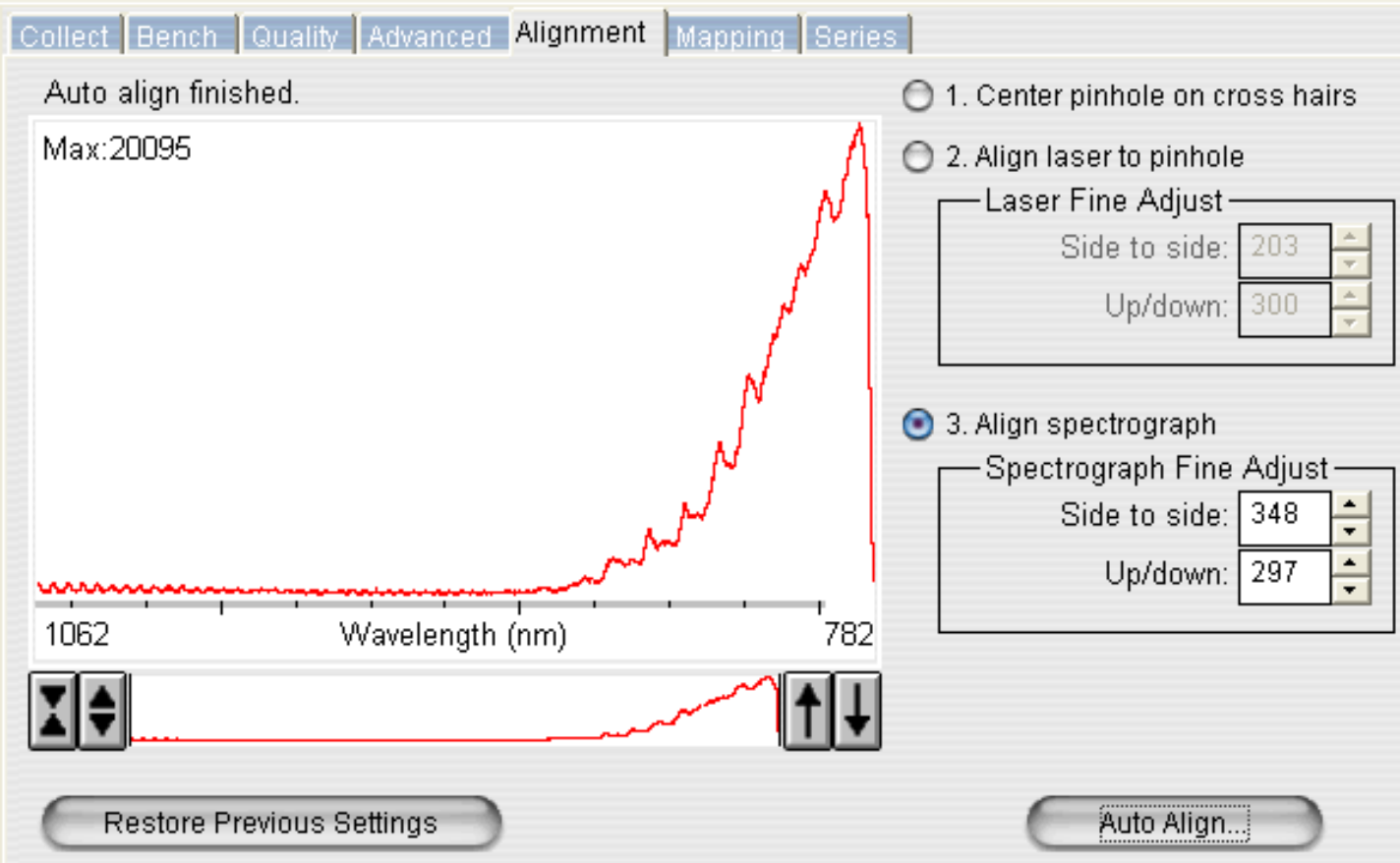
Alignment Tab DXR Raman Microscope

- Align tab will only open if align tool is plugged in
- Customer focuses on pinhole, clicks button 2 and Align
- Laser fine adjusts move to maximize photodiode signal

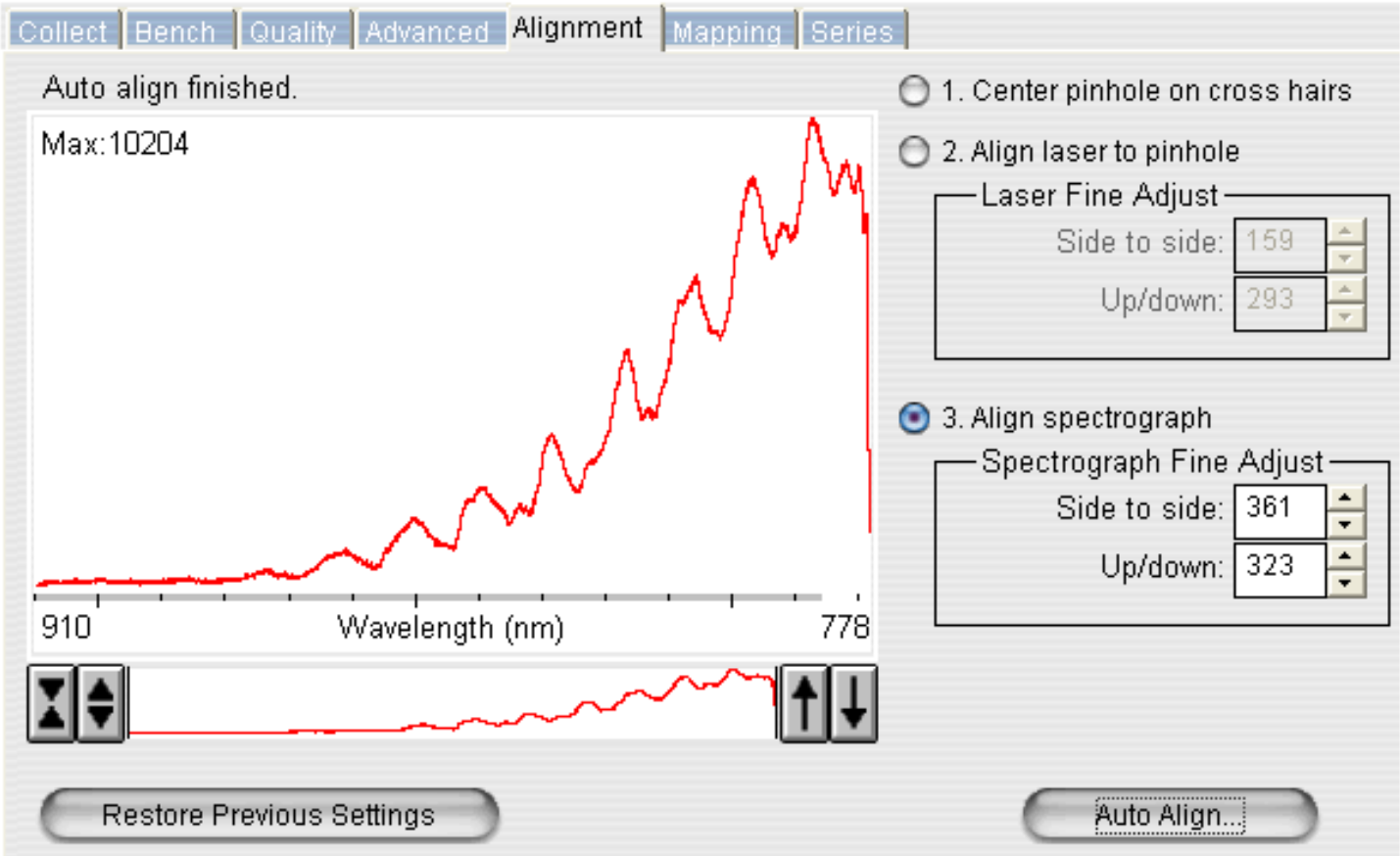


Alignment Tab Microscope (780 full range grating)

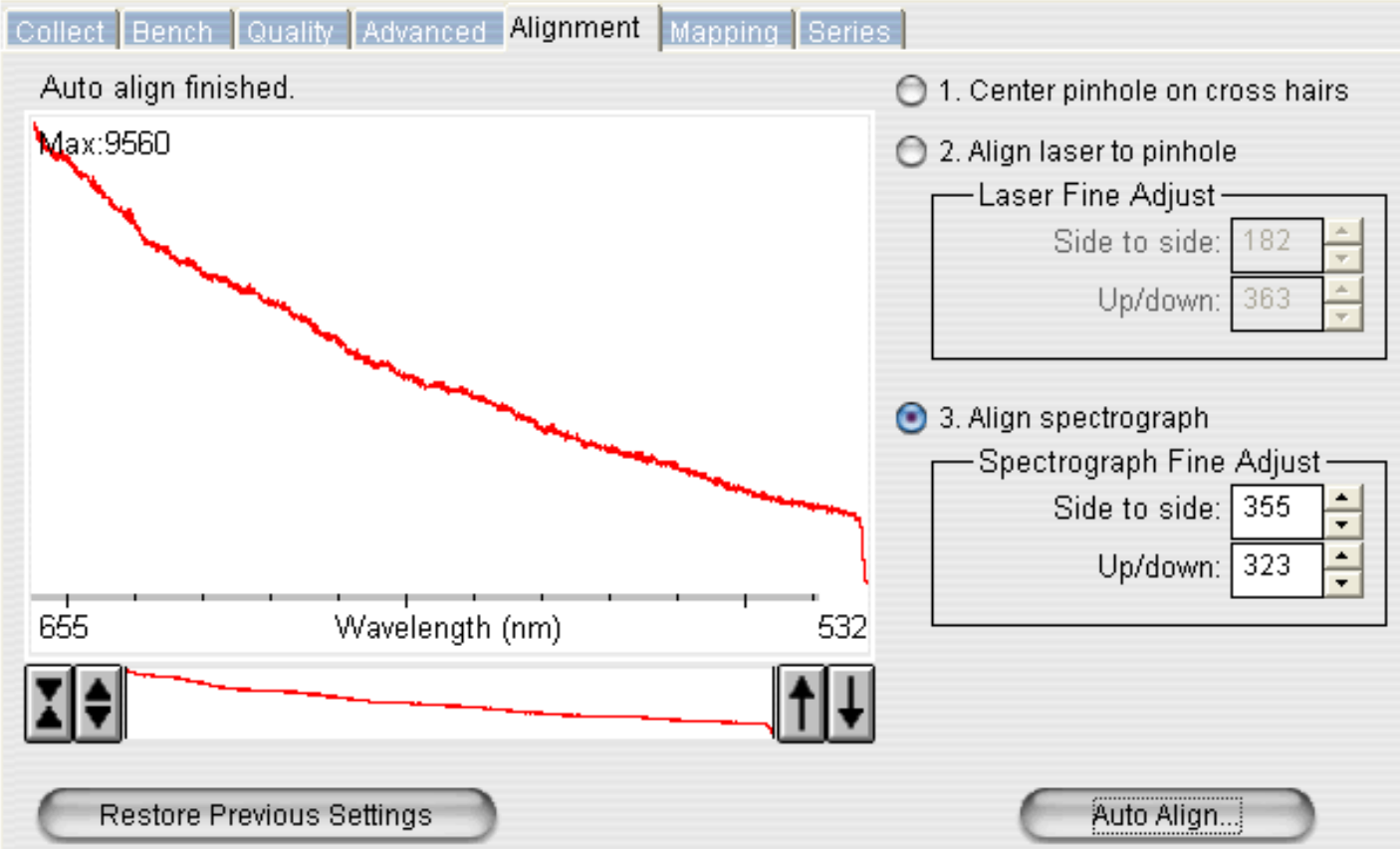
- Step 3, align spectrograph – white light source under pinhole is turned on
- OMNIC moves spectrograph fine adjust lenses to maximize CCD signal
- 780 response is shown below; other lasers and gratings will look different



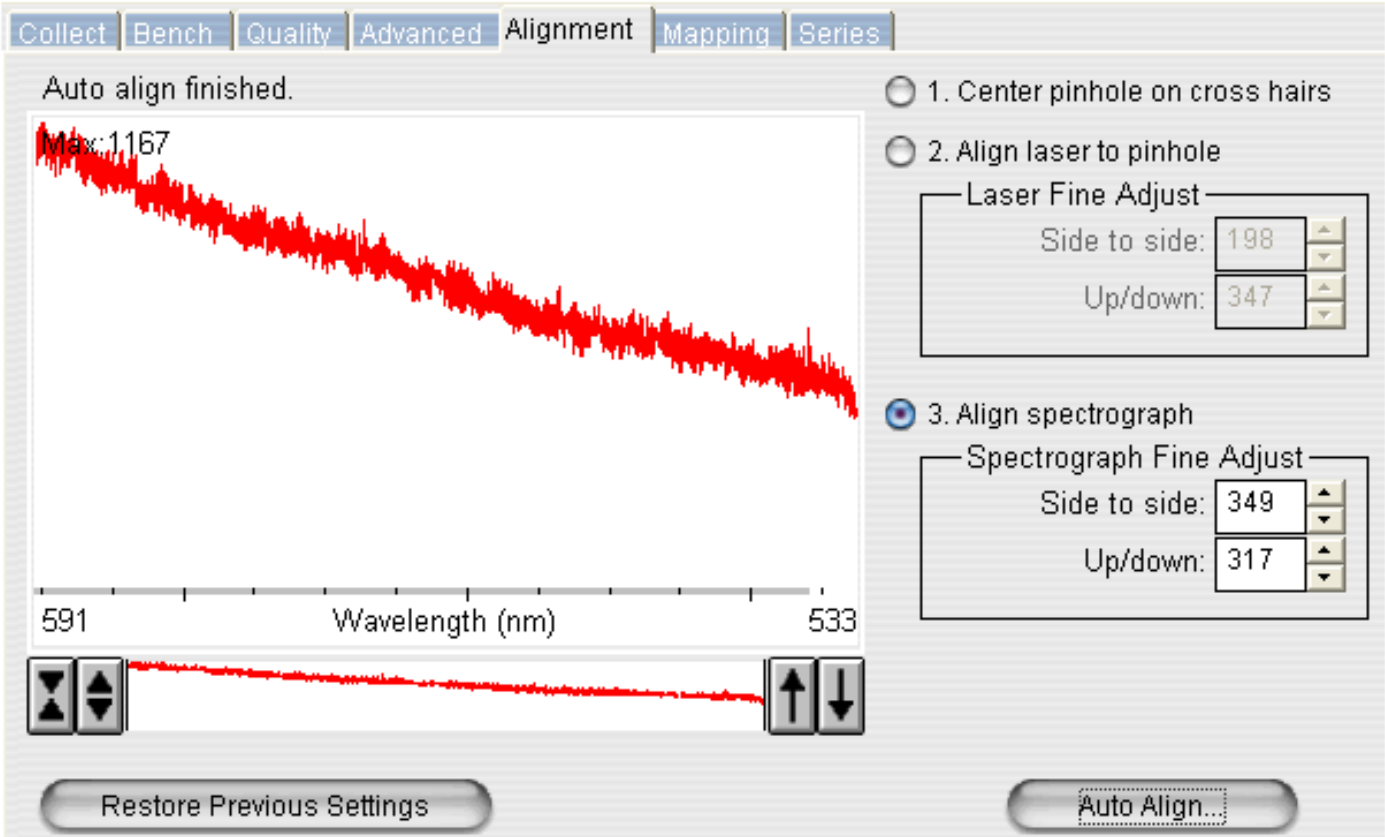
Alignment Tab Microscope (780 high res grating)



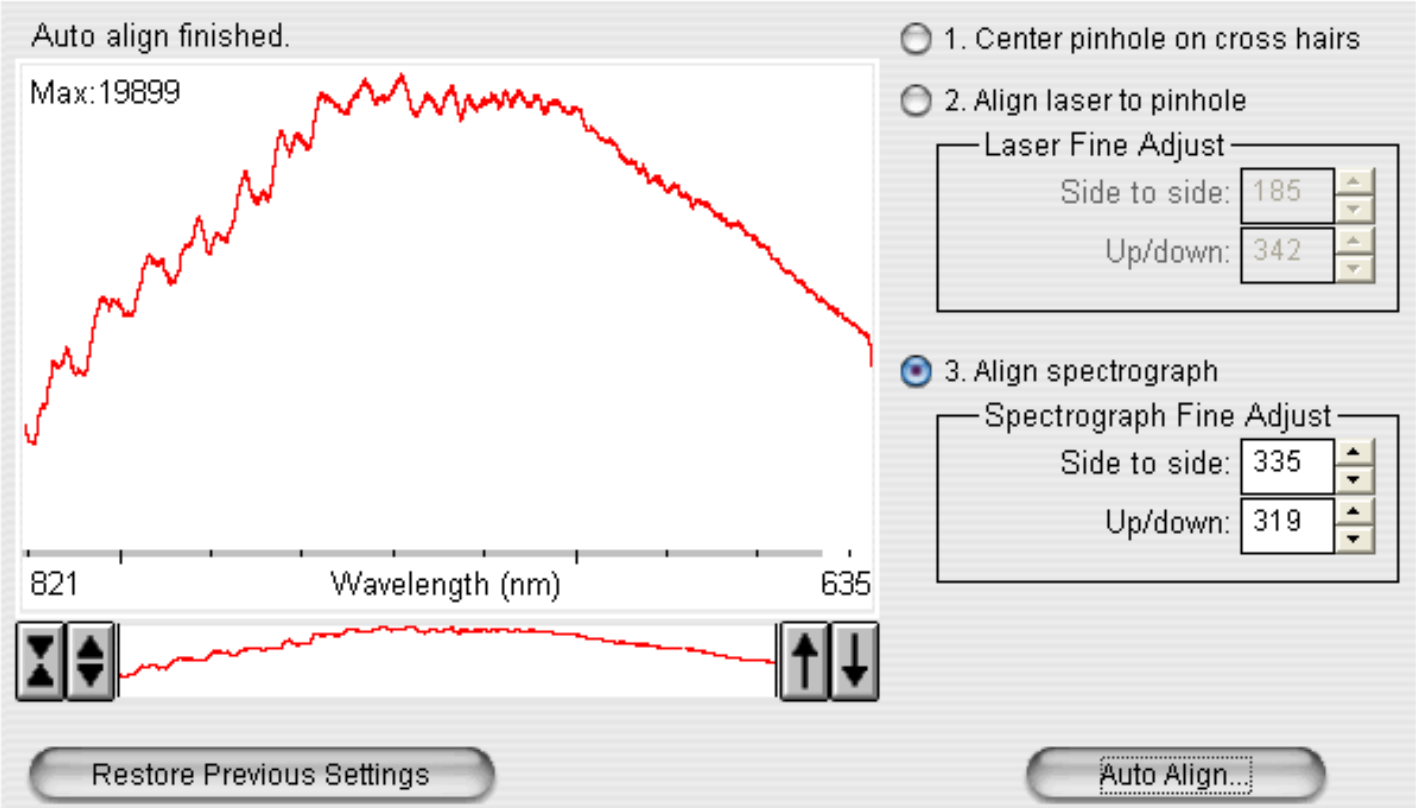
Alignment Tab Microscope (532 full range grating)



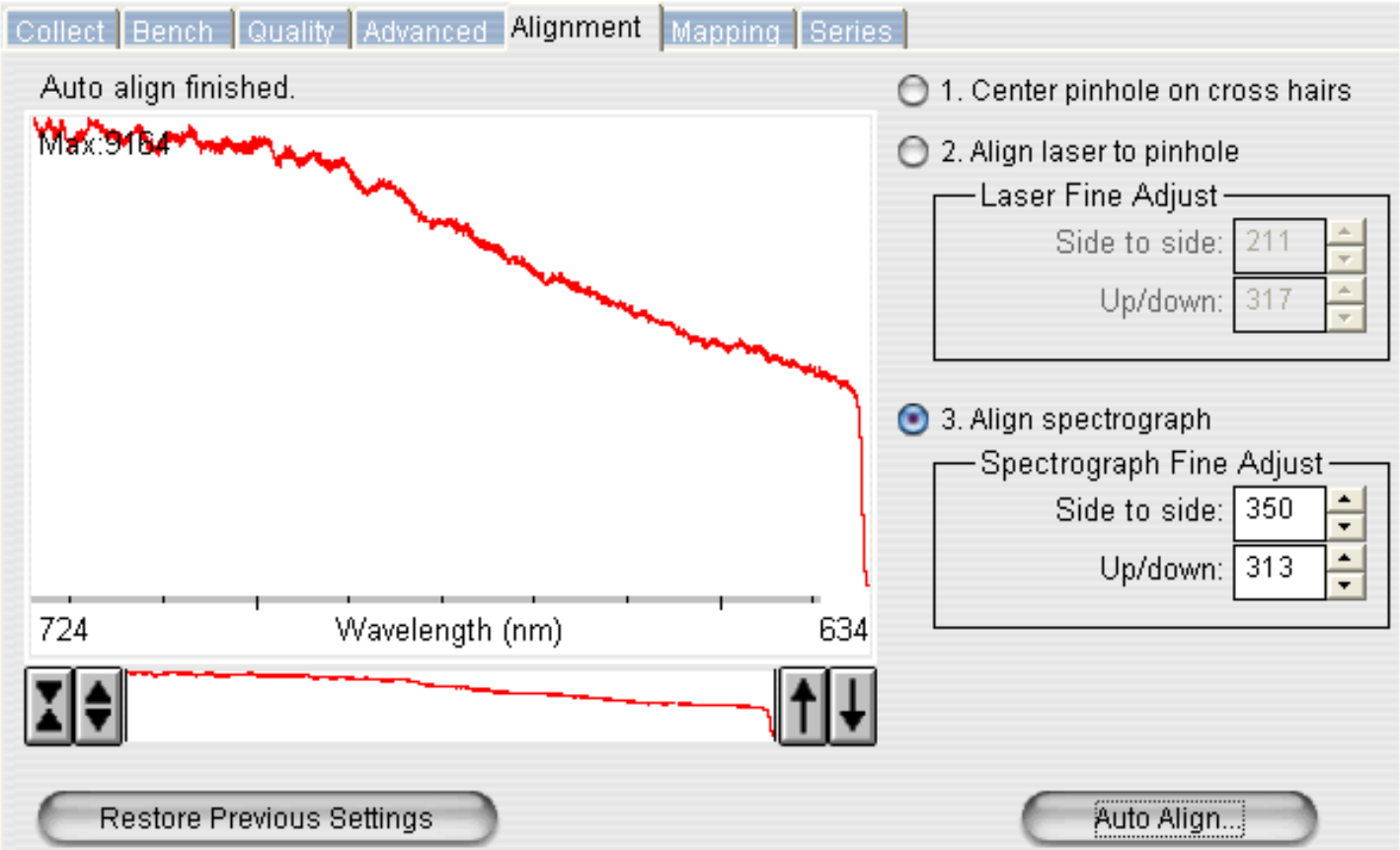
Alignment Tab Microscope (532 high res grating)



Alignment Tab Microscope (633 full range grating)

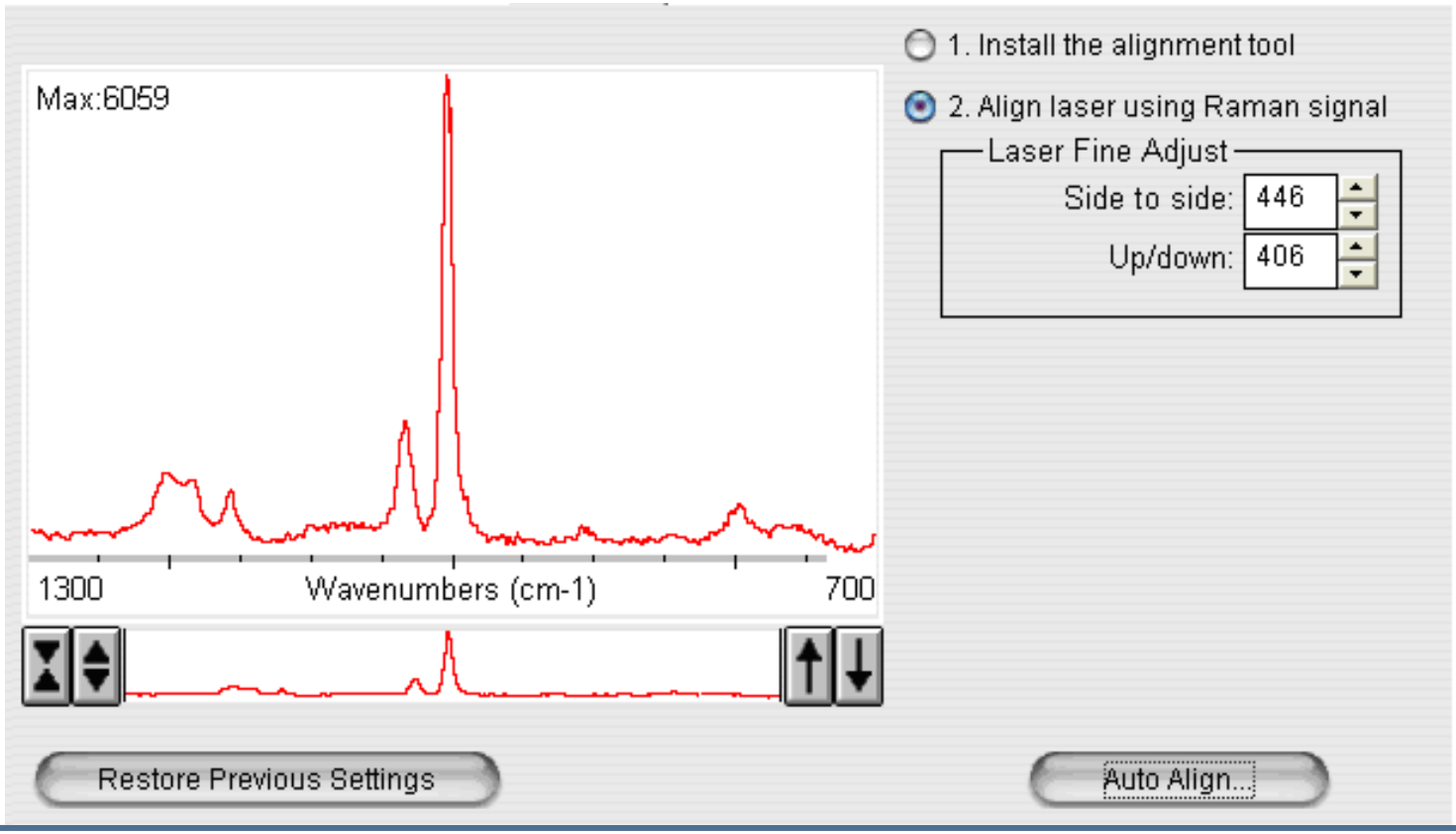


Alignment Tab Microscope (633 high res grating)



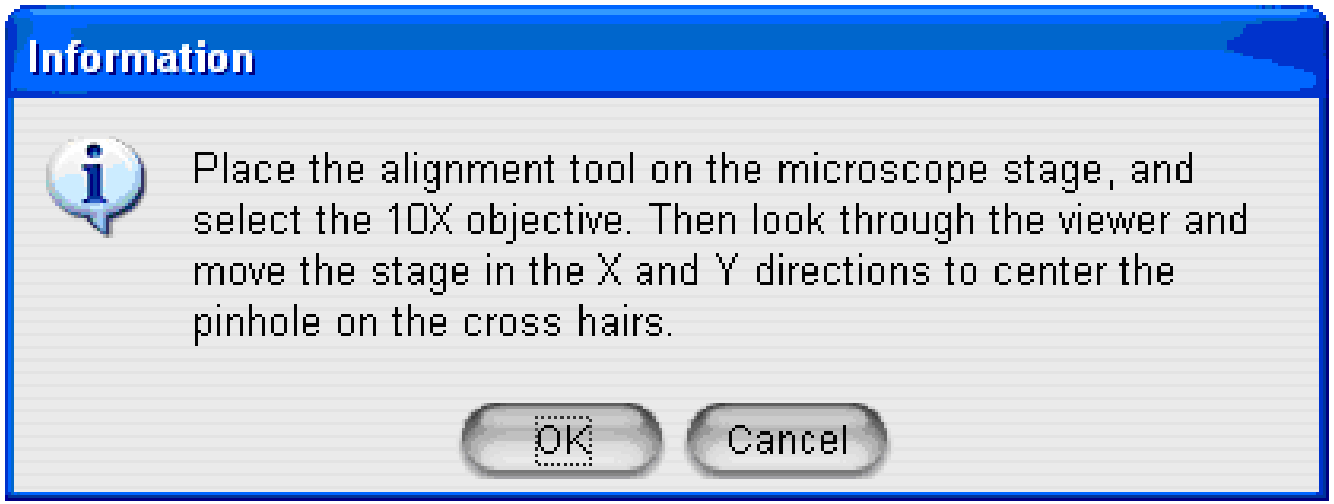
Alignment Tab DXR SmartRaman

- Align tab will only open if macro align tool is inserted
- Customer clicks button 2
- Polystyrene sample inside align tool moves into beam and the laser fine adjusts maximize the 1001.6 cm^{-1} peak



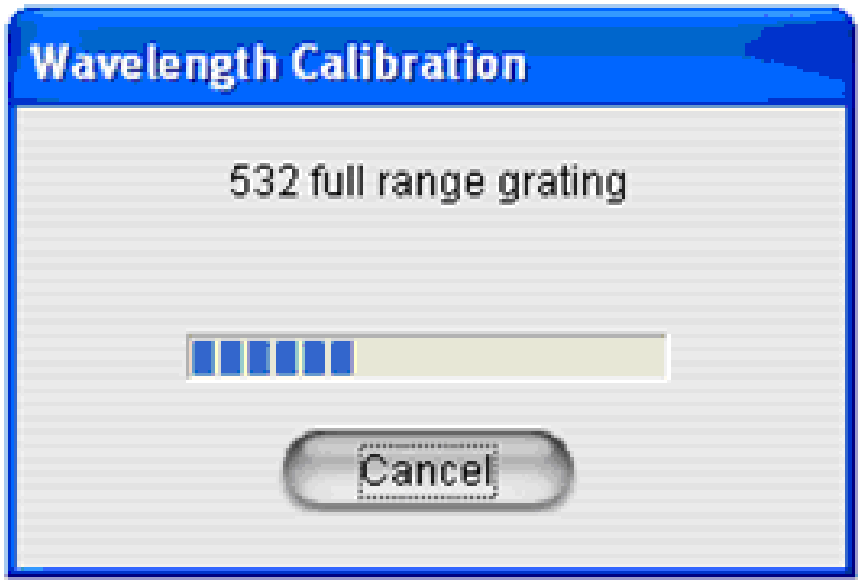
DXR Microscope Spectrometer Calibration

- Select Calibrate Instrument under Collect menu
- Focus and center the pinhole, then click OK



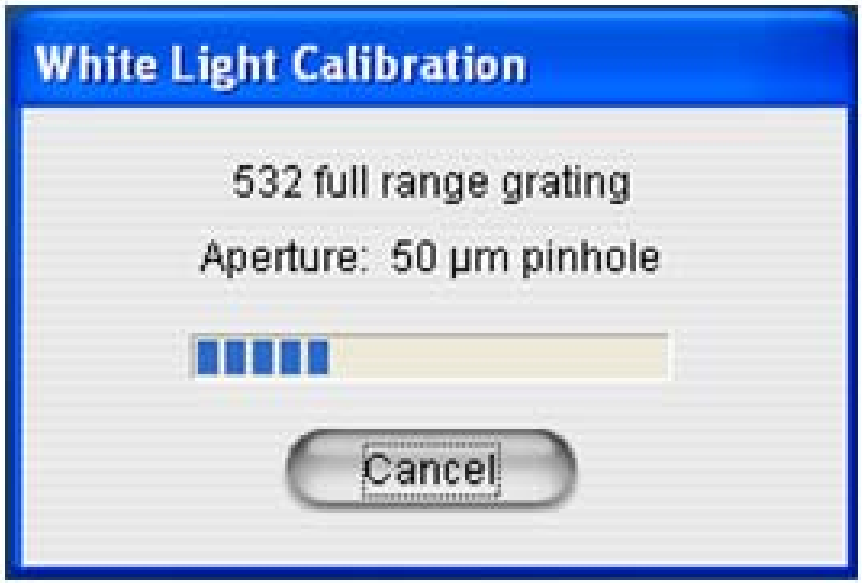
Spectrometer Calibration - Wavelength

- All three calibrations will be performed automatically with no operator intervention.
- Wavelength calibration moves the neon bulb inside the align tool into the beam and uses the emission lines of the neon bulb to calibrate the x-axis. Multiple neon lines are used so that we can correct for offsets and accordion effects.



Spectrometer Calibration – White Light

- White light (intensity) calibration is used to remove the instrument function and give more accurate relative band intensities.
- It uses a white light bulb (or red light if the 780 laser is installed).
- The intensity correction is applied automatically to all spectra.



Spectrometer Calibration – Laser Calibration

- The laser calibration is done by collecting a spectrum from the polystyrene sample inside the alignment tool.
- It compares the measured peak values with the well known polystyrene peak positions and generates a wavenumber correction which is applied to all spectra.

Spectrometer Calibration – Completion

- All three calibrations must pass.
- If the calibrations fail; reseat the grating and filter, align bench and then rerun calibration.
- Laser calibration in order to be successful, needs to have the laser turned on and needs a successful wavelength calibration.