Software User Guide

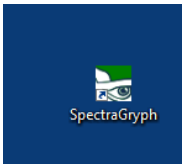
With:

ThunderOptics Spectrometers

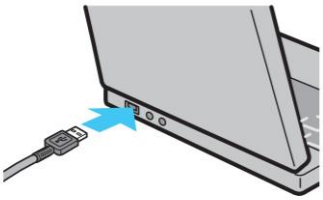
Mini & SMA

Thank you for purchasing ThunderOptics spectrometer. This short manual is to help you using and setting for the first time the ***Spectragryph*** software with our instruments. A full and complete manual of the ***Spectragryph*** software is available online.

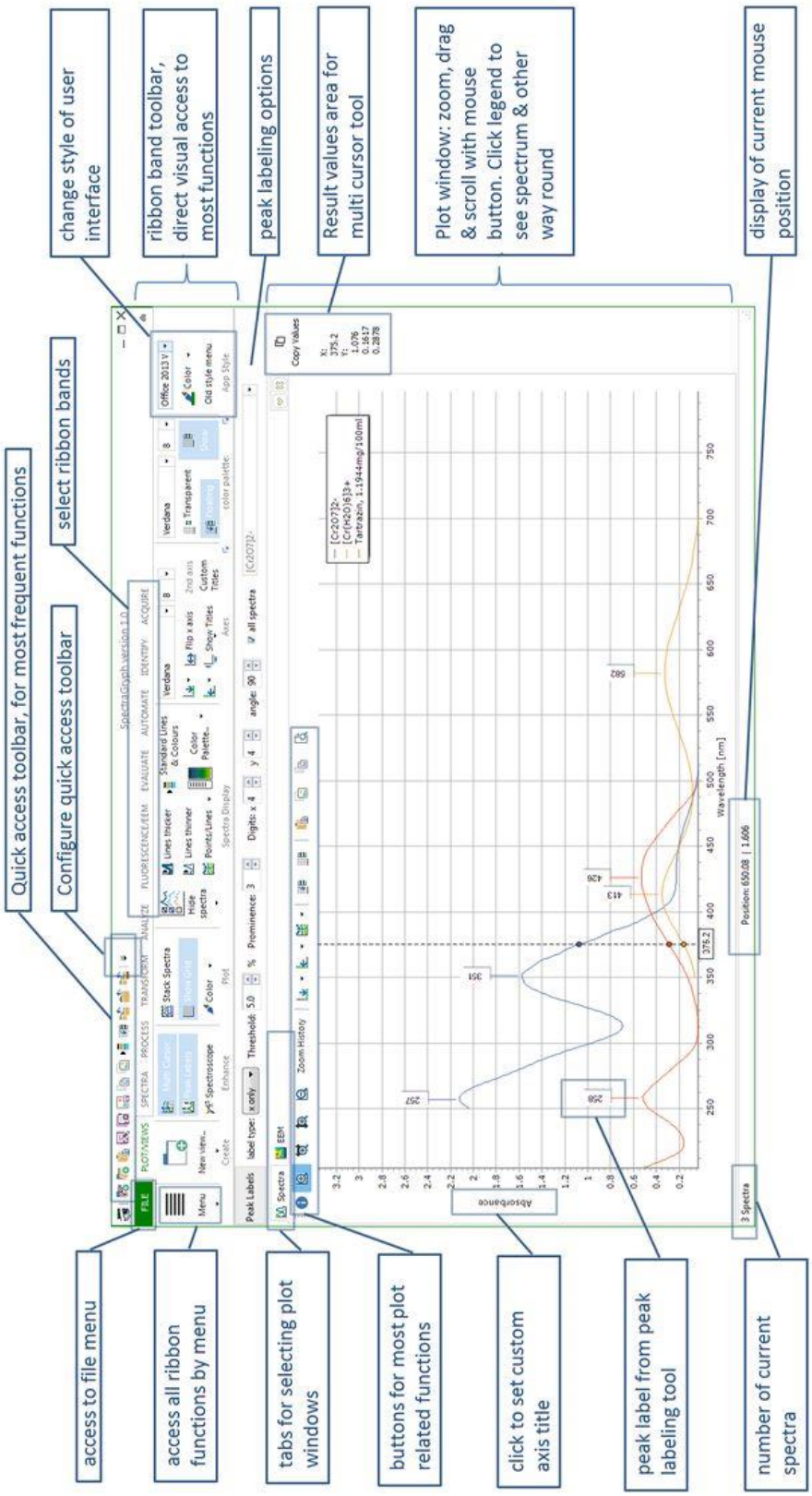
You have received a CD or a download link from ThunderOptics when you purchased your spectrometer. Please, install the executable file and run the software on your computer.



Connect the spectrometer to a USB port of your computer.

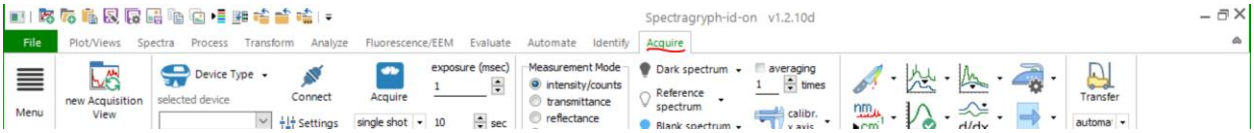


The image in the next page shows the general view of the software interface and explains most of its functionalities.

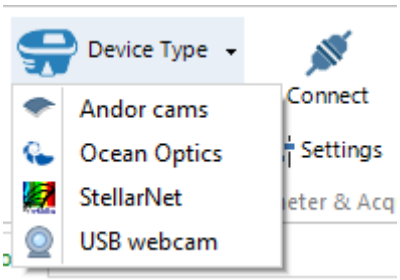

change style of user interface
ribbon band toolbar, direct visual access to most functions
peak labeling options
Result values area for multi cursor tool
Plot window: zoom, drag & scroll with mouse button. Click legend to see spectrum & other way round
display of current mouse position
Quick access toolbar, for most frequent functions
select ribbon bands
Configure quick access toolbar
access to file menu
access all ribbon functions by menu
tabs for selecting plot windows
buttons for most plot related functions
click to set custom axis title
peak label from peak labeling tool
number of current spectra

Spectrometer & Acquisition control

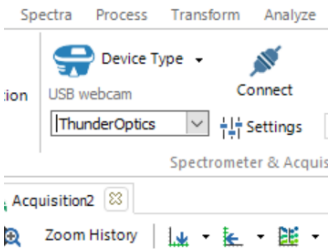
Once the software is open and the USB plug of the spectrometer is connected the “acquire” ribbon band



As a first step, always select the device type from the "Device type" list. Currently, there are: Andor cams, Avantes, OceanOptics, Wasatch Photonics and Stellarnet spectrometer modules and USB webcams.

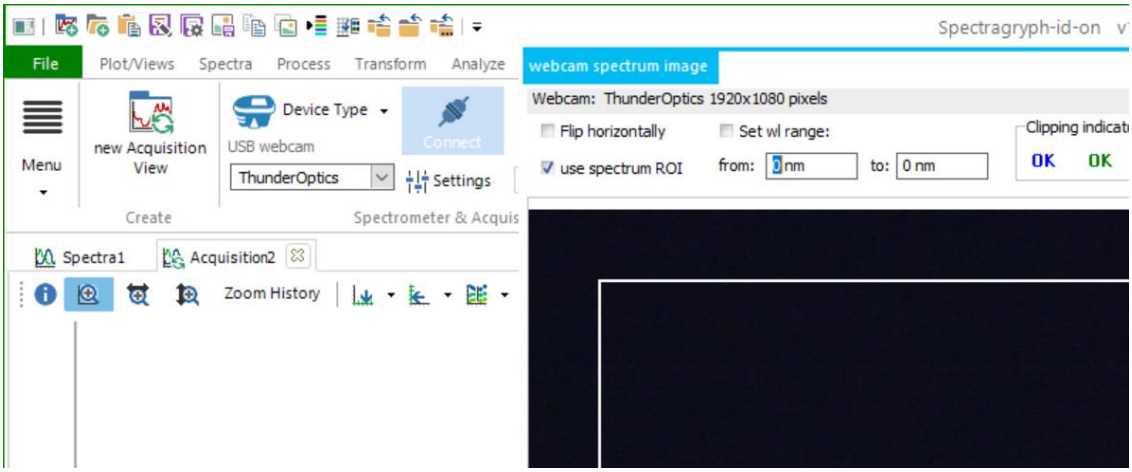


Most of the spectrometers using a *2D detectors are labeled as USB webcams* as they share the fact that they have all 2D (matrix) detector. So, you must *select USB webcam*. And then select ThunderOptics.

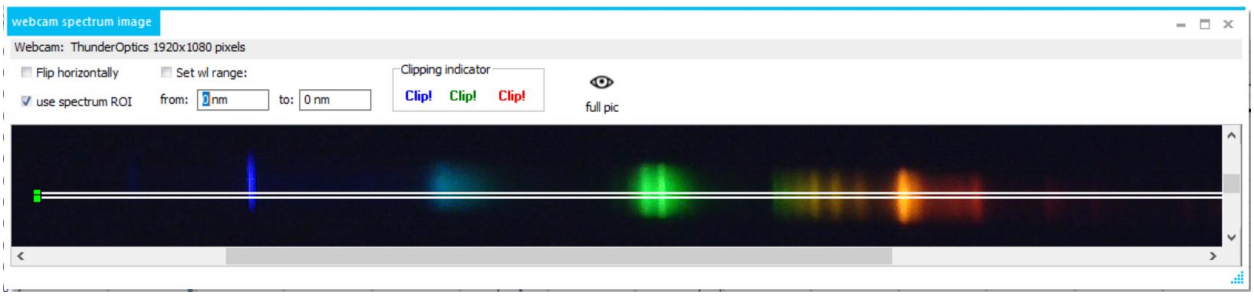


The dropdown list below shows the available devices to select from, if there are more than one devices attached. Only after successful selection of a device type does it make sense to

actually *connect to a device with the [Connect] button*. The connector image will change after successful connection to a "plugged" state. And a new window opens showing the image that send the 2D detector of the spectrometer:

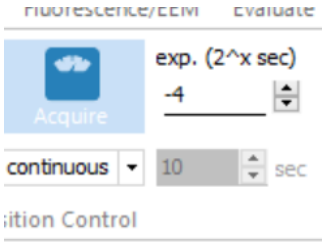


Now, connect a calibration source or shine light to the entrance of the spectrometer (SMA connector for the SMA Spectrometer or the entrance slit for the Mini USB Spectrometer). Adjust the ROI (Region Of Interest) to the size of spectrum.



Note that if the image size is big, the software will take more time to upload it and treat it, and this will slow down the process. Also, in some cases, it is better to have thinner image (in the vertical axis) to have a better resolution.

The desired exposure time can be set anytime (in power of half second) and will apply to the next spectrum acquisition. Note that this option is not available for the low cost Mini USB Spectrometers. In that case the acquisition time is automatically set by the spectrometer.



To acquire live spectra, use the "Acquire" button. This button shows a "down" state only during acquisition, thus it is always visible if there is an acquisition ongoing. Several acquisition modes are possible:

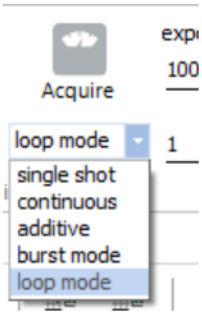
- single shot: grab a single spectrum from the spectrometer, replace the last spectrum in the plot

- continuous: continuing live update of acquired spectra, as fast as exposure time and data transfer allow

- additive: grab a single spectrum from the spectrometer and add it as a new spectrum to the plot

- burst: continuous spectra acquisition, adding them as new spectra to the plot. Process will slow down with present spectra number going up

- loop: continuous spectra acquisition in preset time intervall (use the entry field on the right). To be stopped by pressing [Acquire] button again



Spectrometer settings Settings :

This gives access to multiple parameters at once and allows to save them together as "Spectragryph acquisition settings" file (*.sgas). This file can be loaded again and applied to the currently connected spectrometer.

The upper part give access to parameters that are common to all devices, like exposure time, loop time, acquisition mode and averaging. On the right, there are the calibration coefficients and designated axis types used for x axis calibration. This part is disabled for spectrometers that have their calibration onboard. The lower part of the window gives access to device-specific settings.

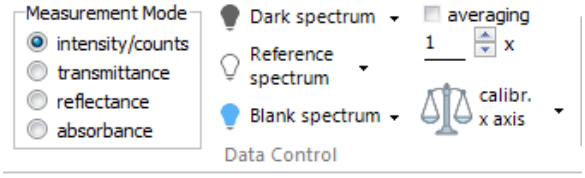
After entering or loading parameters, they can be put to use by clicking the [Apply] button below, or changes can be ignored by closing the window again with the [Close] button below.

The settings can be saved on your computer to upload them when needed with the [Save Settings] button.

Once you have selected the best ROI and acquisition time, you can save the setting and pass to the calibration process of your spectrometers, as the spectrometers come uncalibrated in most cases.

Data control

The selected measurement mode defines the y axis type of the measured live spectrum, with one or more auxiliary spectra needed, depending on the chosen mode. As auxiliary spectrum, there can be dark, reference and Blank spectrum, while each of those can be set, removed and viewed anytime. As soon as these are assigned, they are kept behind the scenes for further use. To update any of them, set them again with a newly measured live spectrum. The dark and the Blank spectrum type are optional, so their use must be activated by clicking onto the respective button. Reference spectrum is mandatory for each y axis type except intensity, so it is used automatically, when necessary.

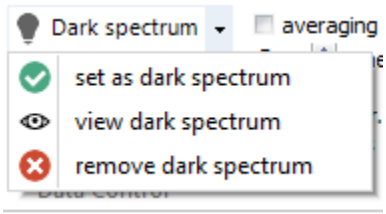


How to measure the auxiliary spectra:

- ***Dark spectrum***: light source off, shutter closed, so that no light falls onto the detector, measurement mode: intensity

- ***Reference spectrum***: light source on, full light (100% level) falling onto the detector, measurement mode: intensity

- ***Blank spectrum***: with blank sample present (like pure solvent or buffer in sample container), with the final measurement mode selected



Each one should be measured again after changing exposure time. Reference should be measured again after any changes in the excitation light intensity.

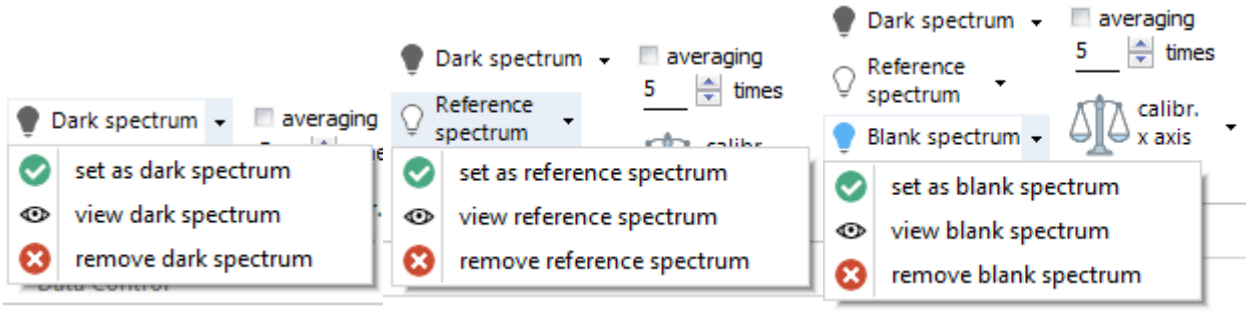
Here are the calculations that happen for the measurement modes, starting with the initially acquired raw spectrum:

intensity/counts: Live = Raw - **Dark** - Blank

transmittance: Live = (Raw - **Dark**) / (**Reference** - **Dark**) - Blank

reflectance: Live = (Raw - **Dark**) / (**Reference** - **Dark**) - Blank

absorbance: Live = - log10 ((Raw - **Dark**) / (**Reference** - **Dark**)) – Blank



Remember: Dark and Blank are used optionally and therefore can be activated/deactivated, while reference is mandatory, therefore transmittance/ reflectance/ absorbance can't be measured without a previously measured reference spectrum. Not all combinations might make sense for all spectroscopy types, you have to know what suits you best. For example, while it might be well advised to subtract both a dark and a blank spectrum in intensity mode for measuring fluorescence intensity, this would make no sense for an absorbance measurement. There, you would subtract the Blank spectrum in absorbance mode. And so on...

If "averaging" is checked, the defined number of raw spectra gets averaged, before being shown as live spectrum.

X axis calibration:

For devices that don't have their calibration on board and give out pixels as x axis data values, an x axis calibration has to be executed. For this, first a light source or sample with known peak positions is measured. Then the measured positions get mapped onto the known positions with polynomial regression. The polynomial coefficients are then ready for use, until the calibration gets invalidated by changes in optical setup or whatever. It is possible to calibrate for

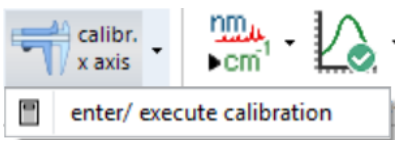
- **Absorbance:** by using a sample with known peaks, like a Holmium or Didymium filter. Target: wavelength scale

- **Fluorescence**: by using a light source with known emission peaks, like a pen lamp source (Hg, Hg/Ar, Xe, Ne). Target: wavelength scale

- **Raman shift:** by using a sample with known Raman lines, as described in ASTM E1840 standard guide. Target: Raman shift scale

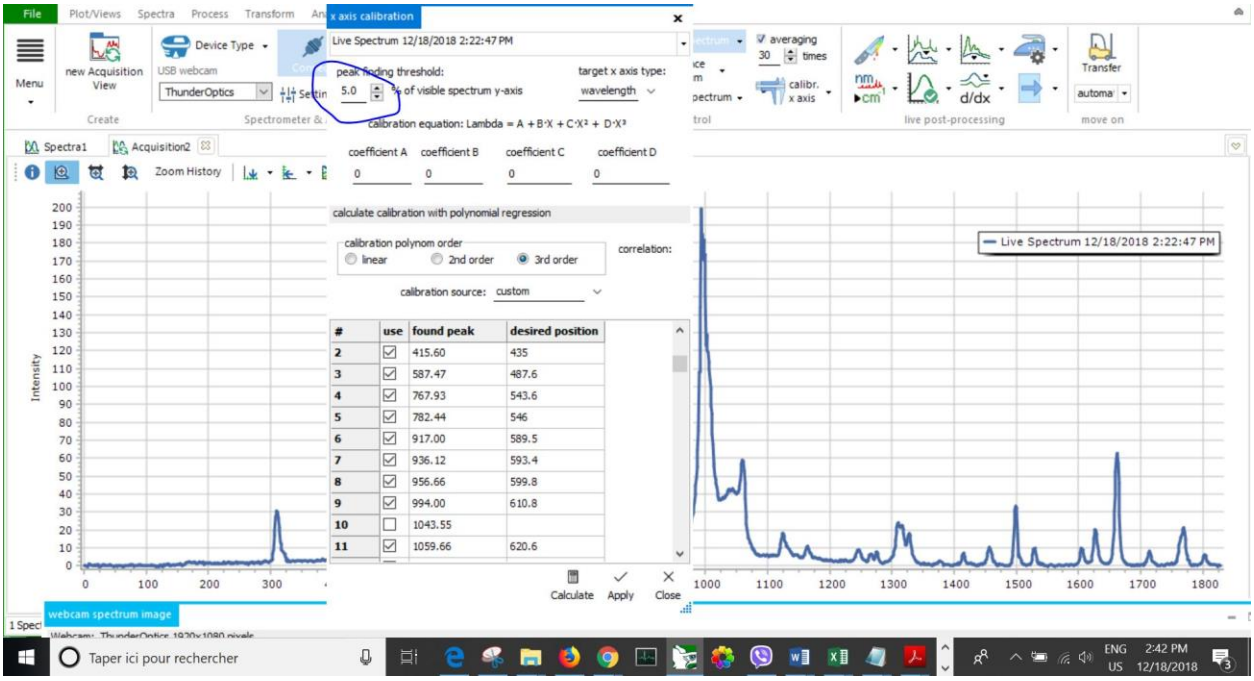
ThunderOptics offers several light sources such calibration sources in the visible or IR and for absorbance/transmittance experiments, please contact us for more information (info@thunderoptics.fr).

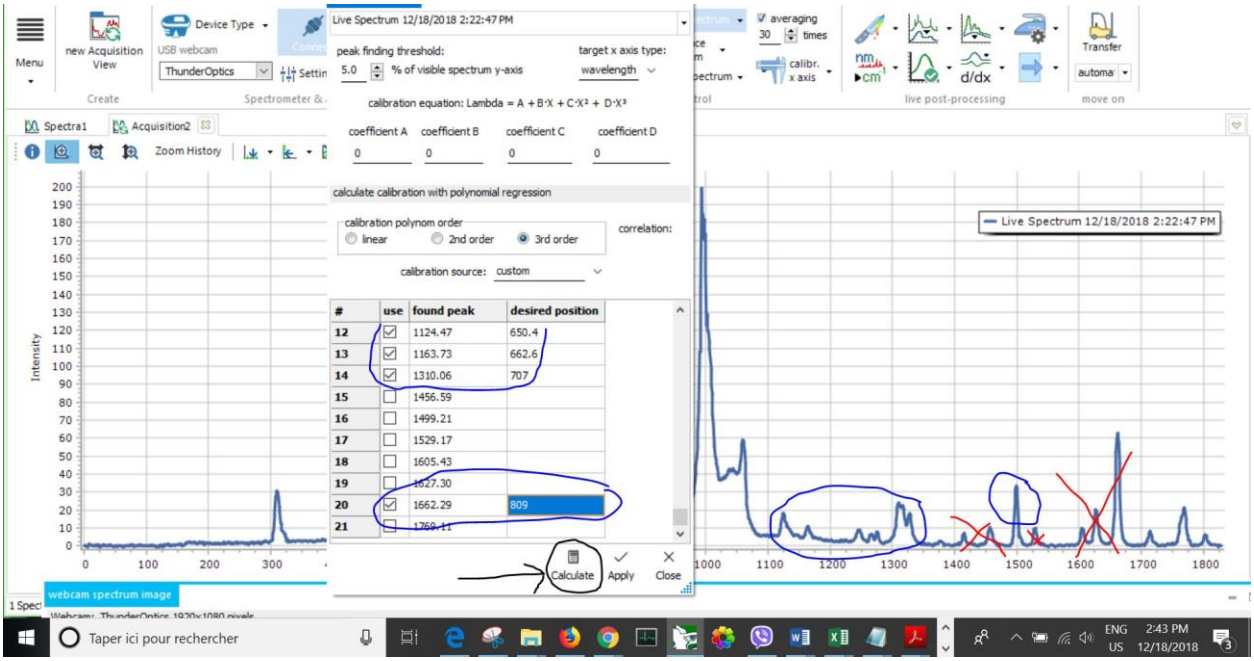
After measuring an appropriate spectrum, open the calibration dialog from the "***calibr. x axis***" button's drop down menu.



In the upper field, select the spectrum to be used. Change the peak finding threshold, if necessary. Select the desired x axis type after calibration on the right side. Below are the fields for the calibration coefficients, that result from the calibration process.

In the table below, the x axis positions of the found peaks from the selected spectrum are displayed. You can either enter the known positions into the "desired position" column manually or select from a number of precompiled positions that are shown as dropdown list. The content of this dropdown list depends on the calibration source chosen above. Only the "custom" option allows to manually enter position values. Check the values to be used during calculation. We give the example of using the fluorescent lamp for calibration to help you select the right peaks.





The best calibration is the have peaks in the whole range from 400nm to 800nm, more extended the range the more accurate will be the calibration. Same for the number of peaks, more you have better will be the calibration.

Finally, select the polynomial order for the regression calculation and press the "***Calculate***" button. The calculated calibration coefficients will show up in the respective fields above. To keep the coefficients and the set target x axis type, use the "***Apply***" button below.

The peak data for the selectable calibration sources is in a file called "calibration_lines.csv" in the program folder, this file's content can be changed to adapt or enhance the range of available calibration peak data.

Turn the calibration-induced axis transformation on/off with the "***calibr. x axis***" button. This can be done on the fly while measuring.

HINT: To better find the peaks to be used during calibration, you might turn on "Peak labels" before starting the calibration procedure.

ANOTHER HINT: The calibration coefficients are saved and loaded together with other settings from the "Settings" dialogue.

ANOTHER HINT: You can lower the peak finding threshold to see more structures and select the real peaks