Program for XMLD and XMCD spectra analysis

User manual

Table of contents

1. Upload tab.

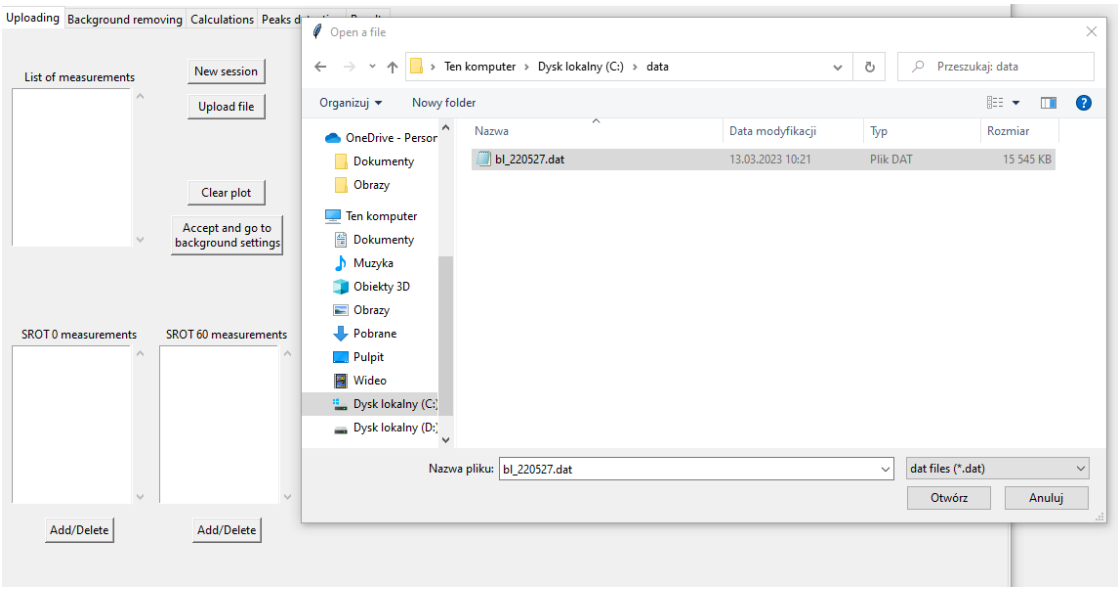

Figure 1. Uploading a file.

1.1. Upload a file.

To upload a file click the button *Upload file* and choose the proper file in the opened File Explorer.

1.2. Choosing measurements for analysis.

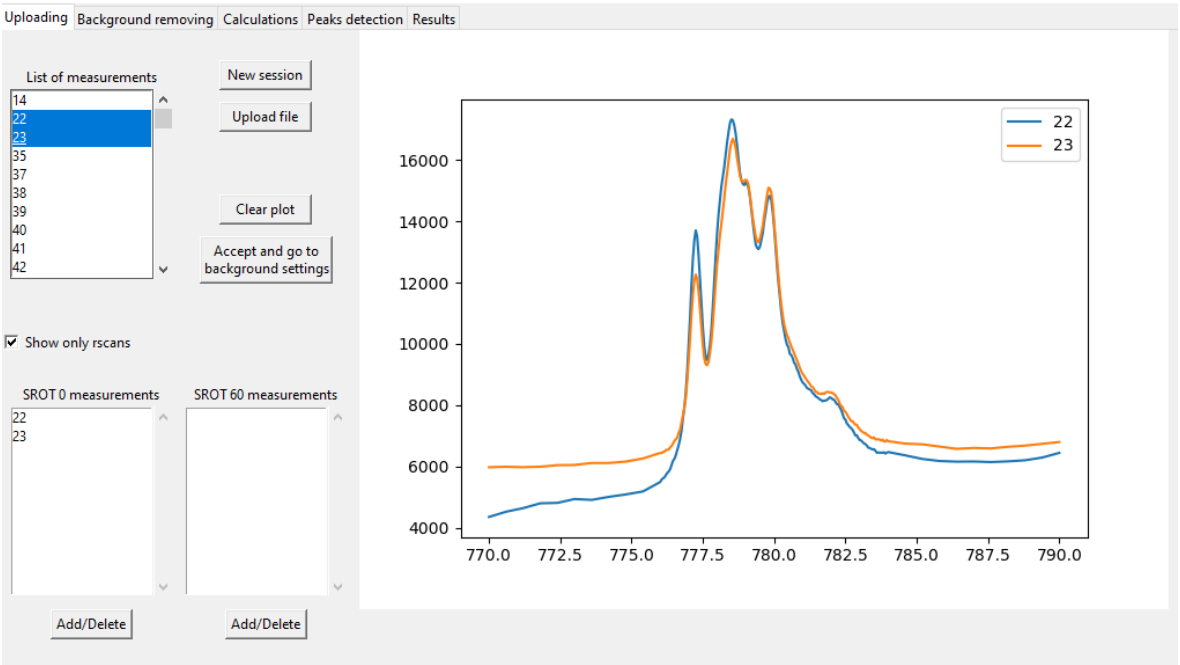

Figure 2. Choosing measurements for analysis.

1.2.1. Show only rscans.

If you want to display only measurements as a function of energy you have to tick *Show only rscans* check button.

1.2.2. Spectrum preview.

To display specific spectra you need to mark the number of proper measurements in the *List of measurements*. To clear the canvas use the button *Clear plot*.

1.2.3. Adding measurements for calculations.

To choose measurements for calculations you need to mark measurements in the *List of measurements* and add them to *SROT 0 measurements* or *SROT 60 measurements* using the proper *Add/Delete* button. Split into two lists allows for calculations for two grazing incident angles (SROT).

1.3. Acceptance of the choices and moving to background removal.

To accept chosen measurements for analysis click the button *Accept and go to background settings*. This will take you to the background removal tab.

2. Background removal tab.

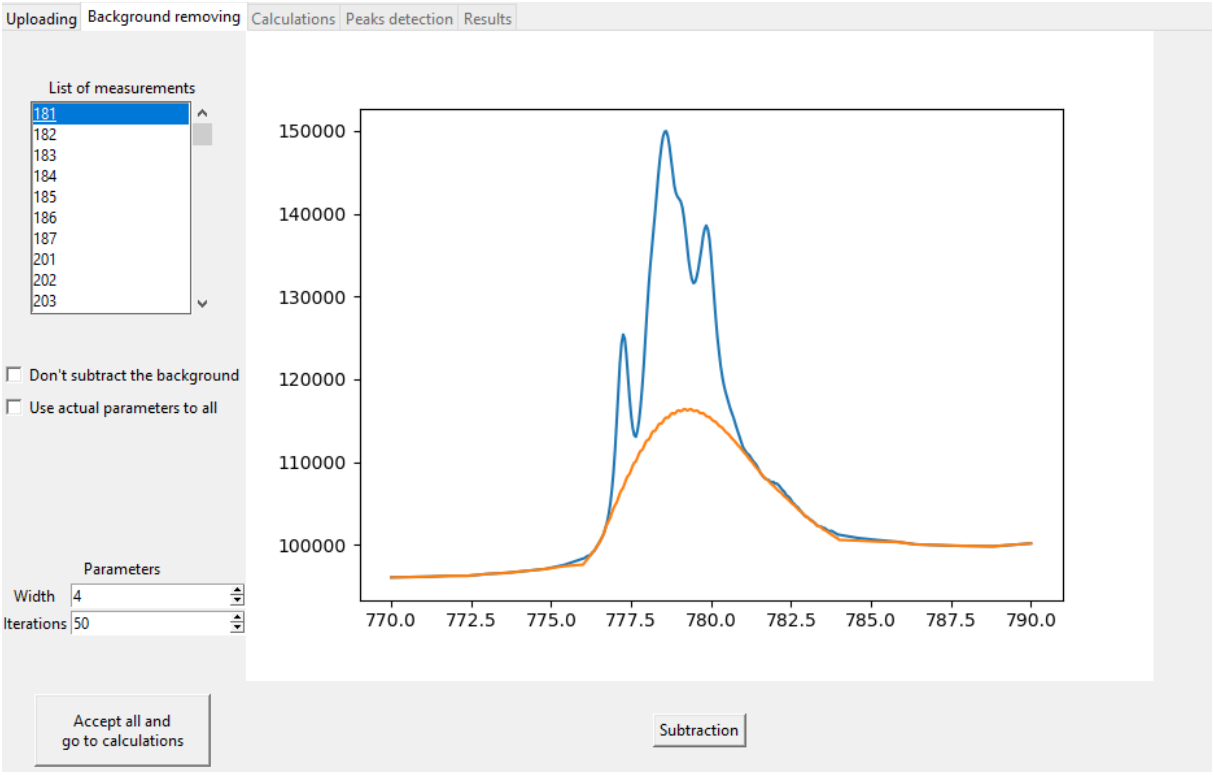

Figure 3. Settings for background removal.

2.1. Background parameters.

You can change the parameters of the background curve fitting in the *Parameters* area. For background fitting the program uses a strip background model that is based on two parameters:

- strip background width (*Width*)
- strip background number of iterations (*Iterations*)

2.2. Settings for background removal.

2.2.1. No background subtraction.

If background subtraction is not necessary tick *Don't subtract the background* check button. The spectra will only be normalized before peaks detection and calculations.

2.2.2. Using the same parameters for subtraction for all spectra.

If you want to subtract background using the same background fitting parameters to all spectra tick *Use actual parameters to all* check-button.

2.2.3. Set parameters of background removal for each spectrum.

If fitting the background using different parameters values to each spectrum is necessary, you have to mark measurement, adjust the parameters, and click the *Subtraction* button.

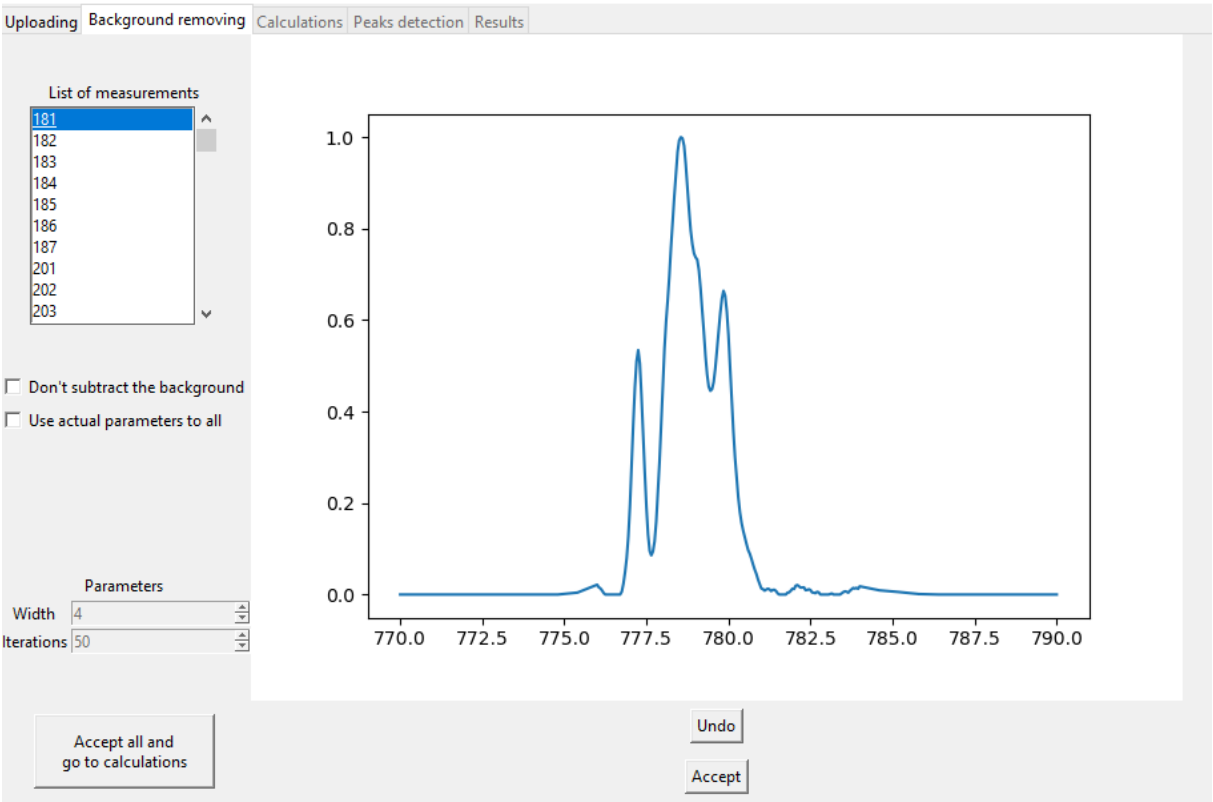

Figure 4. Settings for background removal.

If the fitting parameters turned out to be appropriate click *Accept* button. If you want to change set parameters click *Undo* button.

2.3. Accepting all background settings and moving to the *Calculations* tab.

To approve background removal settings for all spectra, click *Accept and go to calculations* button.

3. Calculations tab.

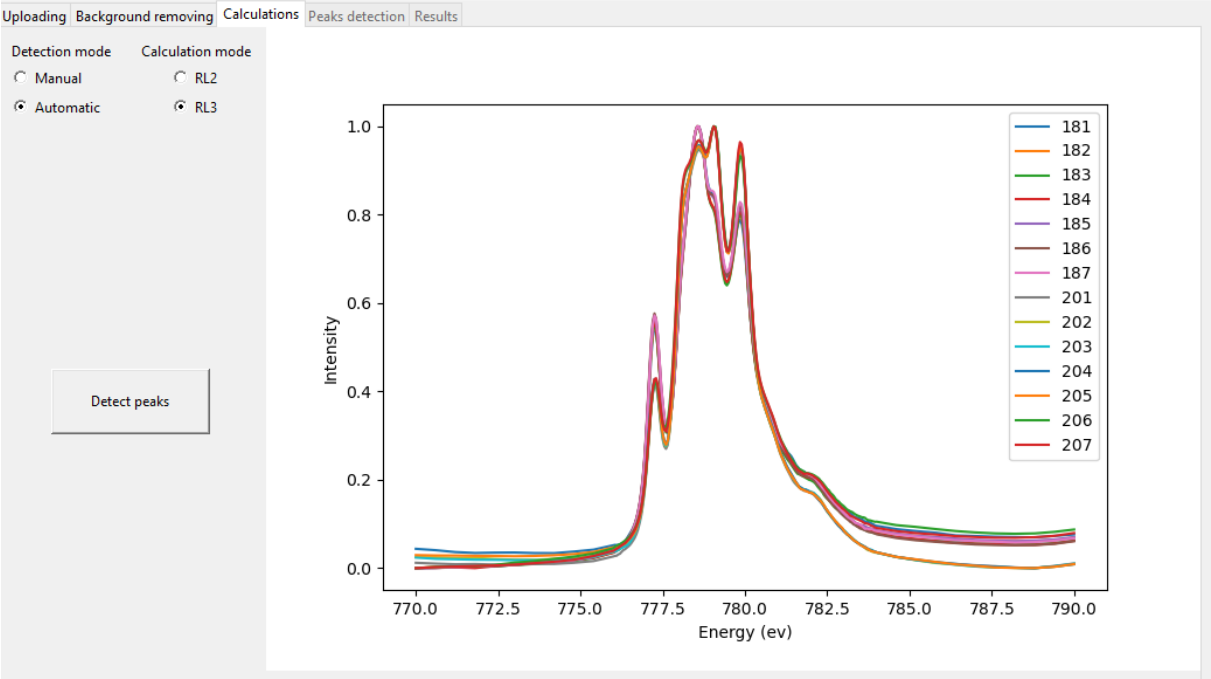

Figure 5. Settings for calculations.

3.1. Plot window.

In the plot window are displayed all spectra after normalization and eventual background removal.

3.2. Choosing detection mode.

3.2.1. Automatic mode.

In automatic mode, peaks will be detected without user input for all spectra unless it is impossible to detect peaks using the program algorithm for any of the spectra.

3.2.2. Manual mode.

In manual mode have to mark peaks by picking points on the plot for each of the spectra.

3.3. Choosing calculations mode.

3.3.1. RL2 mode.

RL2 and ΔRL2 coefficients will be calculated for all spectra.

3.3.2. RL3 mode.

RL3 and delta ΔRL3 coefficients will be calculated for all spectra.

3.4. Moving to the detection of the peaks.

To start the detection of the peaks with chosen modes click the *Detect peaks* button.

4. Peaks detection tab.

4.1. Peaks detection in automatic mode.

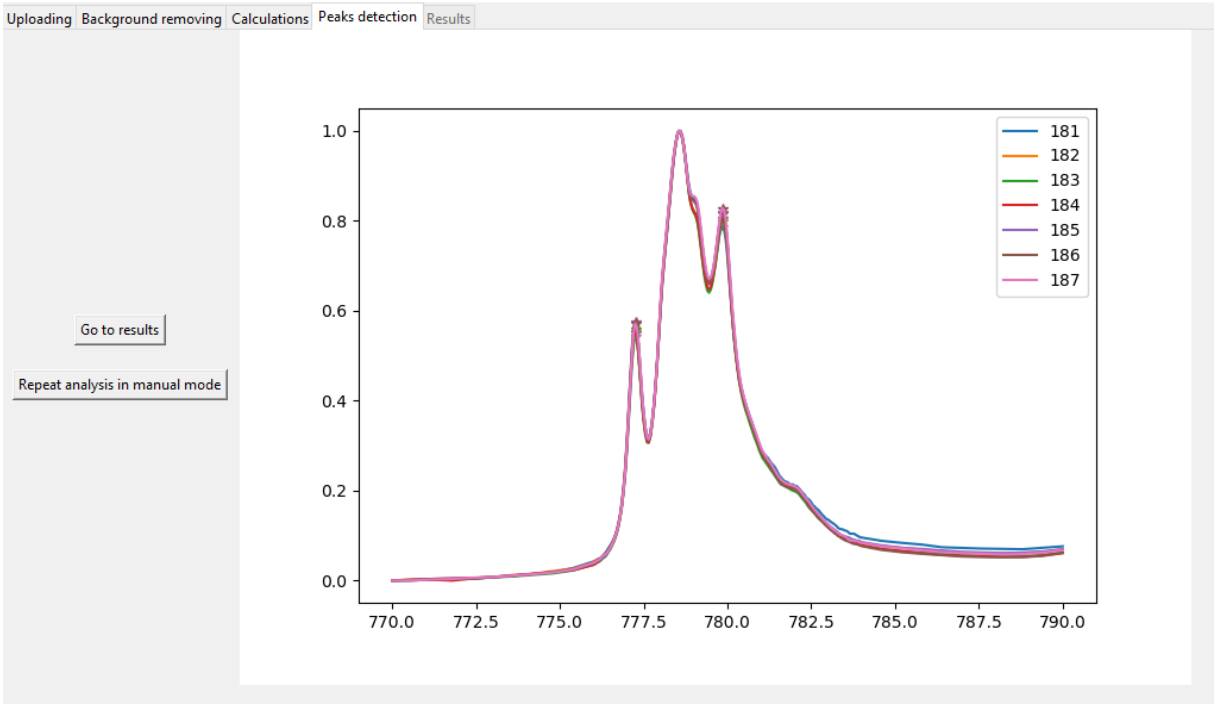

Figure 6. Peaks detection tab for automatic mode.

4.1.1. Displaying detection results.

When the automatic mode was chosen, after going to the detection section all spectra with marked two detected peaks will be displayed in the plot window.

4.1.2. Repetition of the detection.

If detection results are unsatisfactory you can repeat the analysis in manual mode using the *Repeat analysis in manual mode* button.

4.1.3. Accepting automatically searched peaks and moving to the results tab.

If detection results are satisfactory click the *Go to results* button. It will result in acceptance of all peaks and moving to the Results tab.

4.2. Peaks detection in manual mode.

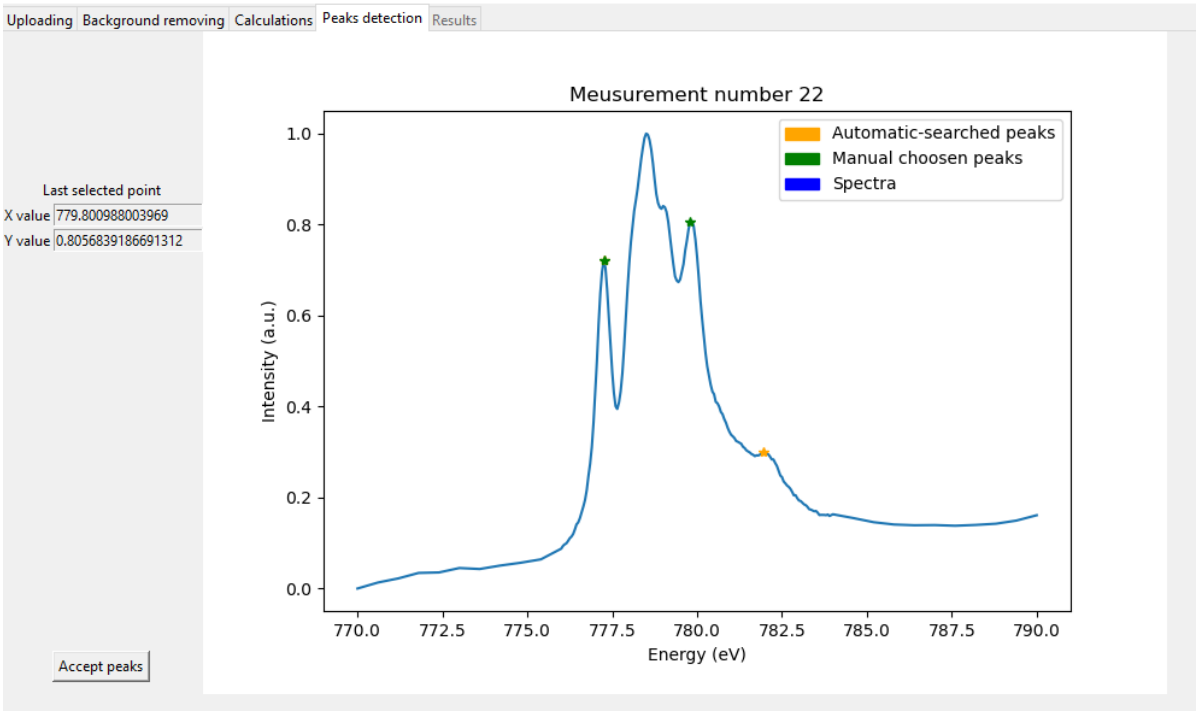

Figure 7. Peaks detection tab for manual mode.

4.2.1. Displaying detection results.

Spectra are displayed one by one in the plot window with marked two detected peaks. After considering each of the spectra, all spectra with manually chosen peaks will be displayed.

4.2.2. Choosing positions of peaks.

If automatic detection results are satisfactory you can accept it by clicking the *Accept peaks* button. In another case, you can choose the position of two peaks manually by left-clicking on the plot. Coordinates of the last selected point will be displayed in the *Last selected point* area. You can delete the last selected point by right-clicking. If you are satisfied with your choices, click the *Accept peaks* button. It will result in the acceptance of peaks chosen for the actual spectrum and moving to the next spectrum.

4.2.3. Accepting manually chosen peaks and moving to the results tab.

After accepting peaks for the last spectrum all spectra will be displayed with marked peaks. You can repeat detection or accept detection results and move to the *Results* tab (see paragraph 4.1.3.)

5. Results tab.

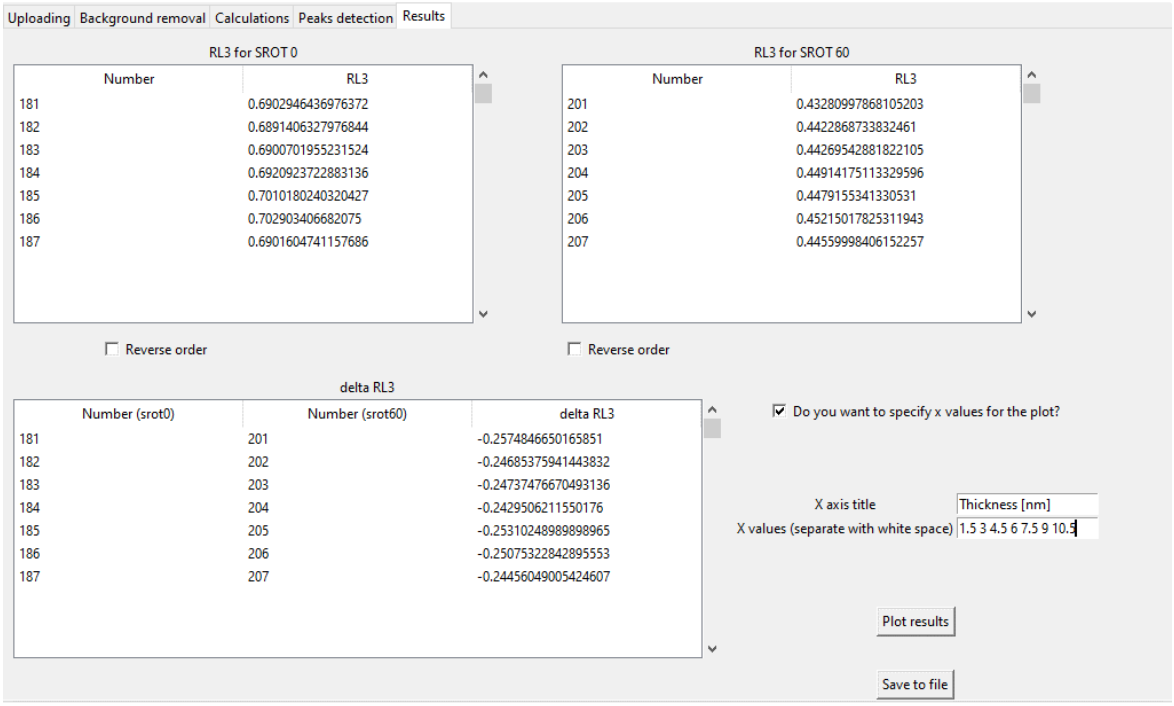

Figure 8. Results tab – presentation of results.

5.1. Displaying results.

5.1.1. Tables with data.

All calculated RL and ΔRL coefficients will be displayed in the tables with corresponding signatures.

5.1.2. Changing order of the measurements.

To reverse the order of measurements in one of the RL tables, mark proper *Reverse order* check button. It induse changes in the ΔRL table, plots and file with saved results.

5.1.3. Graphical presentation of results.

To plot the results use the *Plot results* button. The program will create four plots:

- All spectra after normalization and background removal
- RL coefficient for SROT 0
- RL coefficient for SROT 60
- ΔRL coefficient

If you want to specify X values and axis title for the RL and ΔRL plots, tick *Do you want to specify x values for the plots?* check button and provide data in the form shown in Figure 8.

5.2. Saving the results.

To save the results to a CSV file (UTF8) click the *Save to file* button. It will result in the opening of File Explorer where you can specify the name and localization of the file.