

What is new in UNIFIT 2018?

In order to have more linking options for the fit parameters the fit procedures were improved. The selection of the master peaks of the peak fit with relative fit parameters was extended. The main-memory used by UNIFIT was reduced with a new definition of the large parameter arrays. A fourth method was implemented in the new software. Next to photoelectron spectra (XPS), Auger electron spectra (AES) and X-ray absorption spectra (XAS) Unifit 2018 offers the data analysis for RAMAN spectra.

- i) In former versions of the UNIFIT software the definition of the master peak of the peak fit with relative fit parameters was fixed and settled to the first component. Now, every peak-fit component can be defined as master peak. The parameters of slave peaks with a higher component number can be linked to the parameters of the corresponding master peak. A colour code in the fit-parameter table informs the operator of the component status:

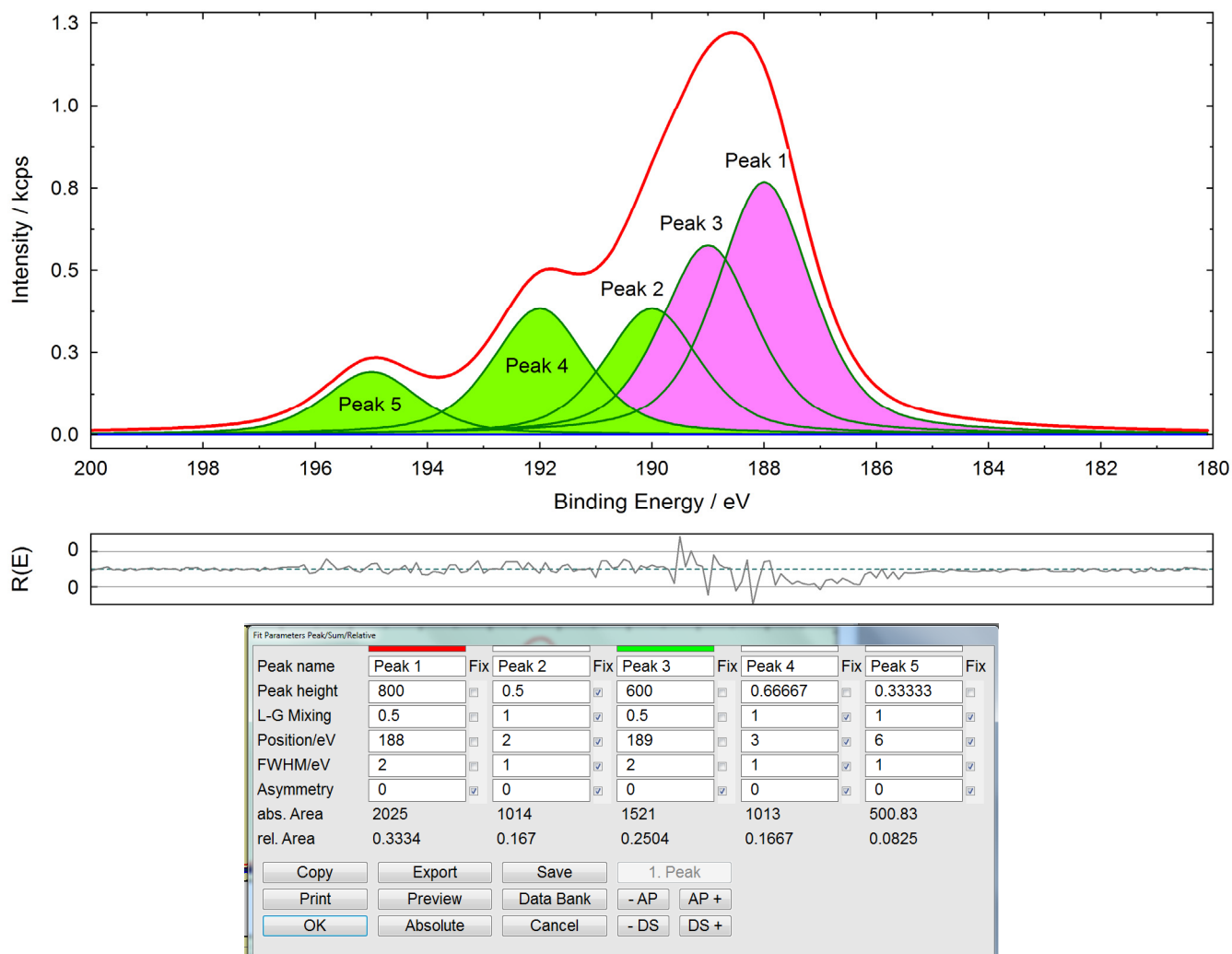


Fig. 1. Top: Peak fit of a test spectra with five components, bottom: Fit-parameter table of five single peaks of the test spectrum, fit conditions: sum of Gaussian and Lorentzian peaks, relative fit-parameters, peak 1 and peak 3 defined as master peaks, peak 1 activated for input, parameters of peak 2 are relative to the parameters of peak1, parameters of peak 4 and peak 5 are relative to the parameters of peak 3

RED: Master peak, activated for input,
 GREEN: Master peak, not activated for input,
 BLUE: Slave peak, activated for input,
 WHITE: Slave peak, not activated for input (Fig. 1).

The XPS-background parameters for inhomogeneous samples and the XAS-background parameters may be defined in the same way.

- ii) The main-memory used by UNIFIT was strongly reduced. The UNIFIT 2018 software needs more than 30% less main-memory with respect to UNIFIT 2017. The large parameter arrays were redefined.
- iii) The peak identification for XP spectra was expanded by an automatic option. The peak-finding procedure can be approached by defining of ΔE (energy separation), ΔI (peak height) as well as a check with a data set of main lines (see Fig 2). The annotation list may be shown directly.

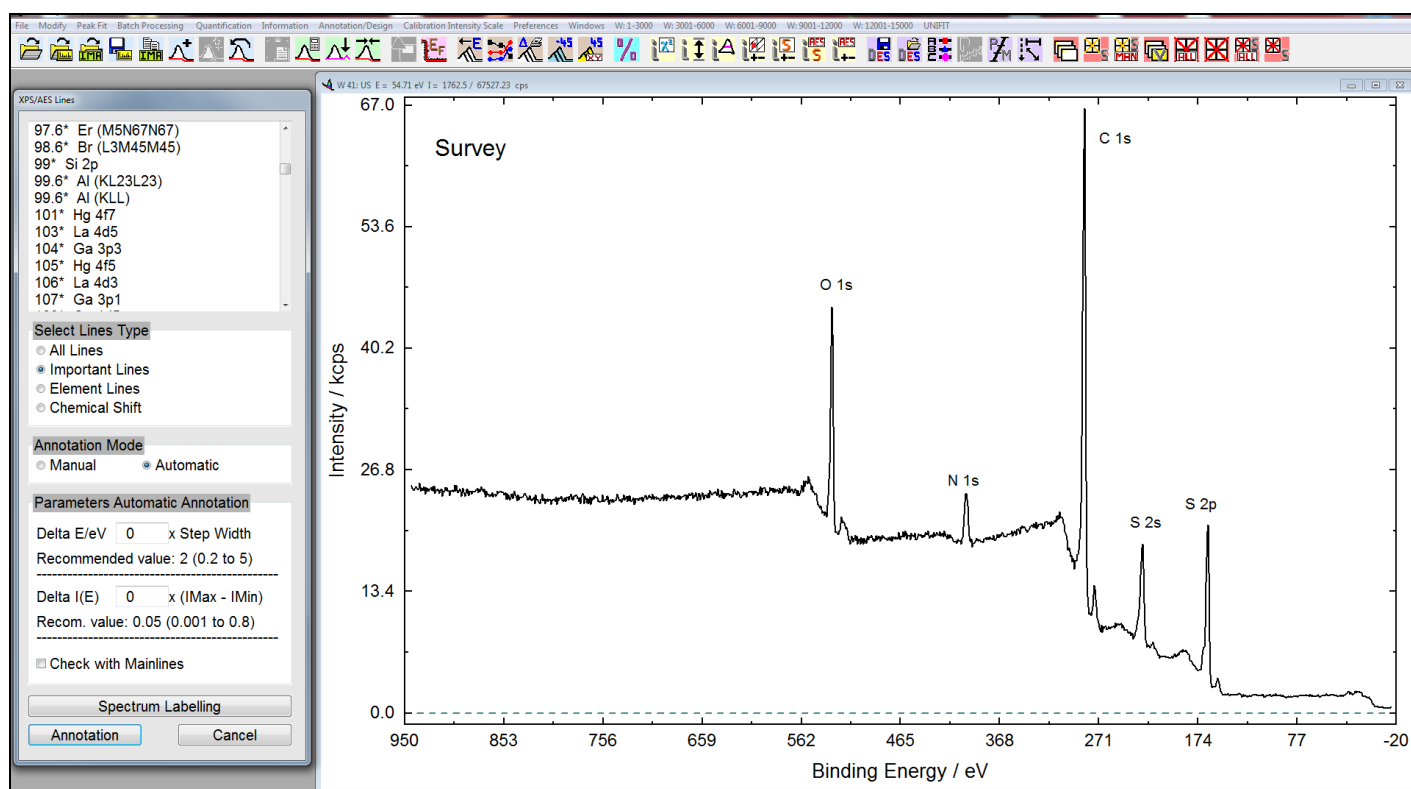


Fig. 2. Screen shot: right: Survey spectrum, left: dialogue of the improved submenu 'Identify Lines' for XPS, the file 'Mainlines.pos' can be modified directly using UNIFIT 2018

- iv) The sequence of the plot of the peak-fit components can be changed without a modification of the sequence of the components of the peak-fit procedure (see Fig. 3).
- v) Two new 3D plots were implemented in the batch processing subroutines. The presentations 'XY 3D 45° Colour Profile' and 'XY 3D -45° Colour Profile' are combination of the presentations 'XY 3D Colour Profile' and 'XY 3D Plot 45°' as well as 'XY 3D Colour Profile' and 'XY 3D Plot -45°'. Figure 4 illustrates the new programme features using a RAMAN-multipoint measurement.

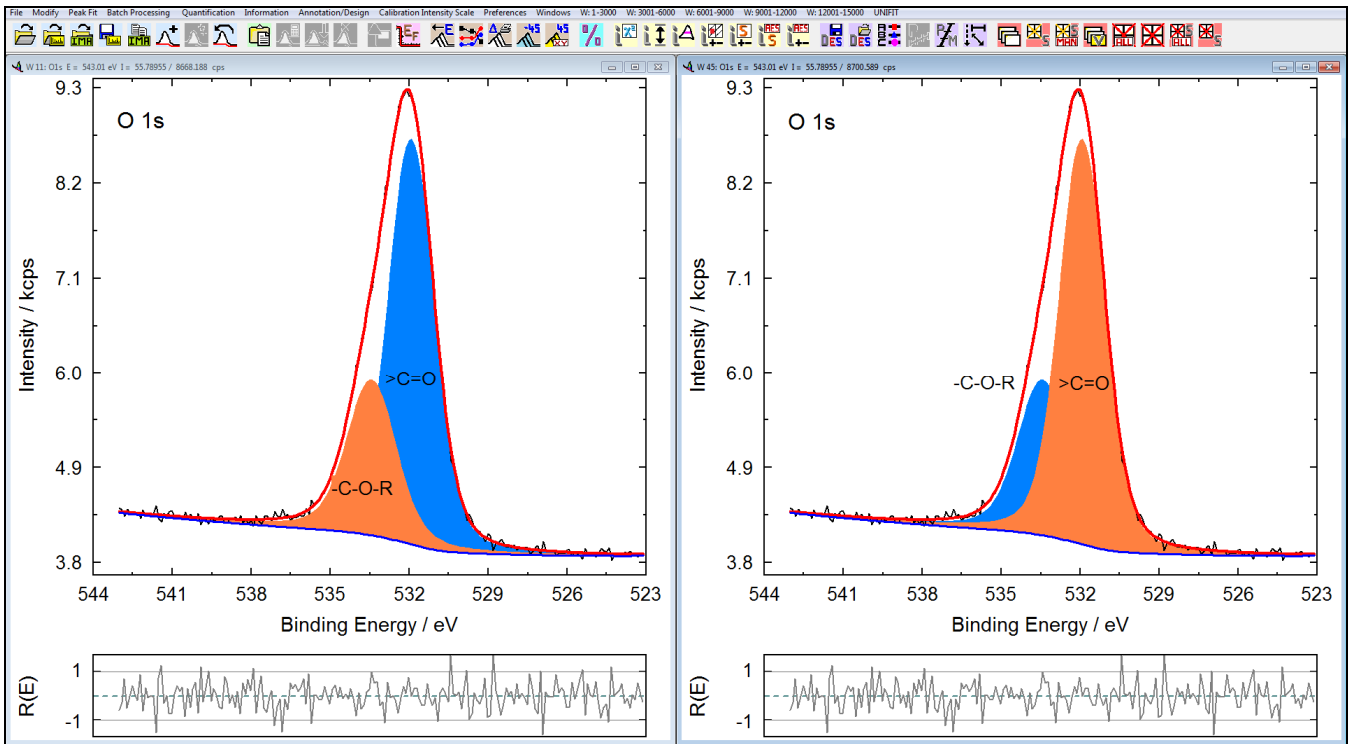


Fig. 3. Screen shot: peak fit of O 1s with two components, left: first peak-fit component is plotted behind the second, right: second peak-fit component is plotted behind the first

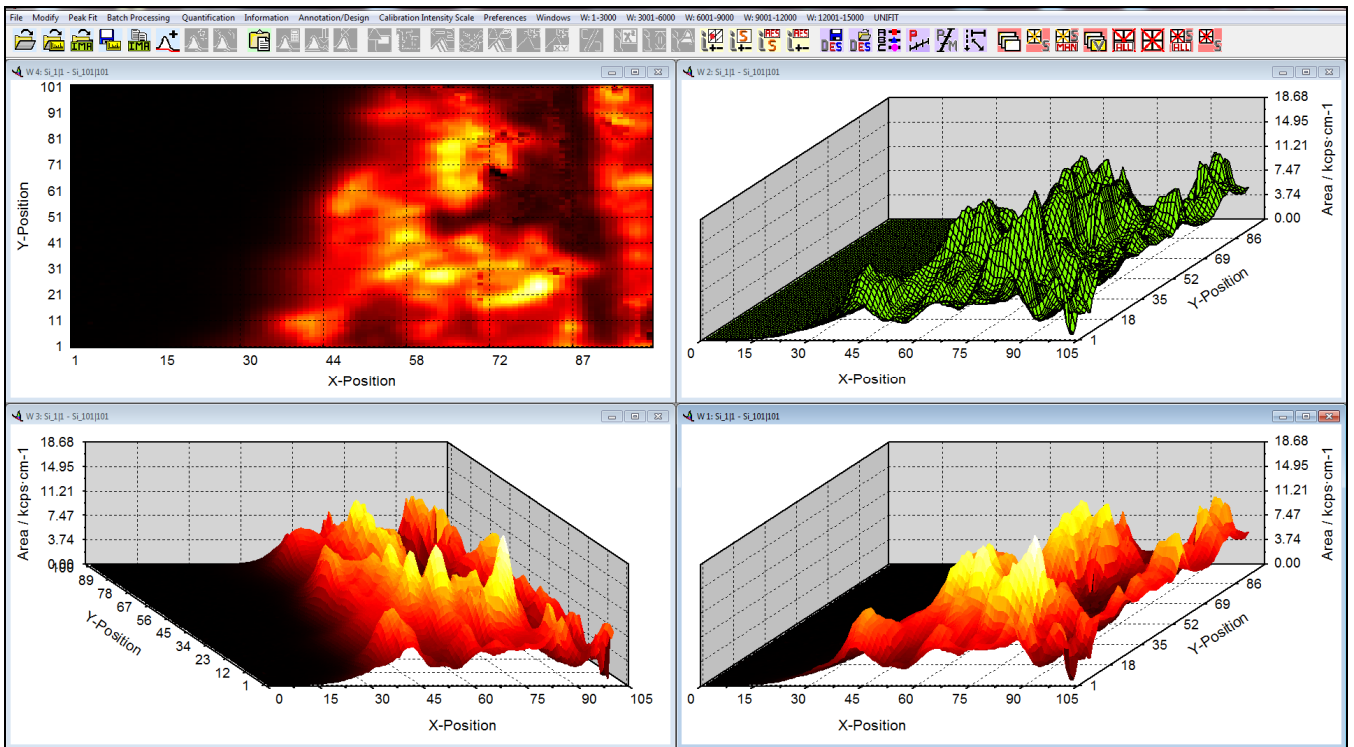


Fig. 4. Screen shot: presentations of the estimated peak area of the Si signal using peak fit of a RAMAN-101x101-multipoint measurement, top left: 'XY 3D Colour Profile', top right: 'XY 3D Plot 45°', bottom left: 'XY 3D -45° Colour Profile', bottom right: 'XY 3D 45° Colour Profile'

vi) The selectable processing results for the generation of XY-3D presentations were enhanced. Now, all fit parameters, the position of the maximum and minimum can be selected additionally (Fig. 5).

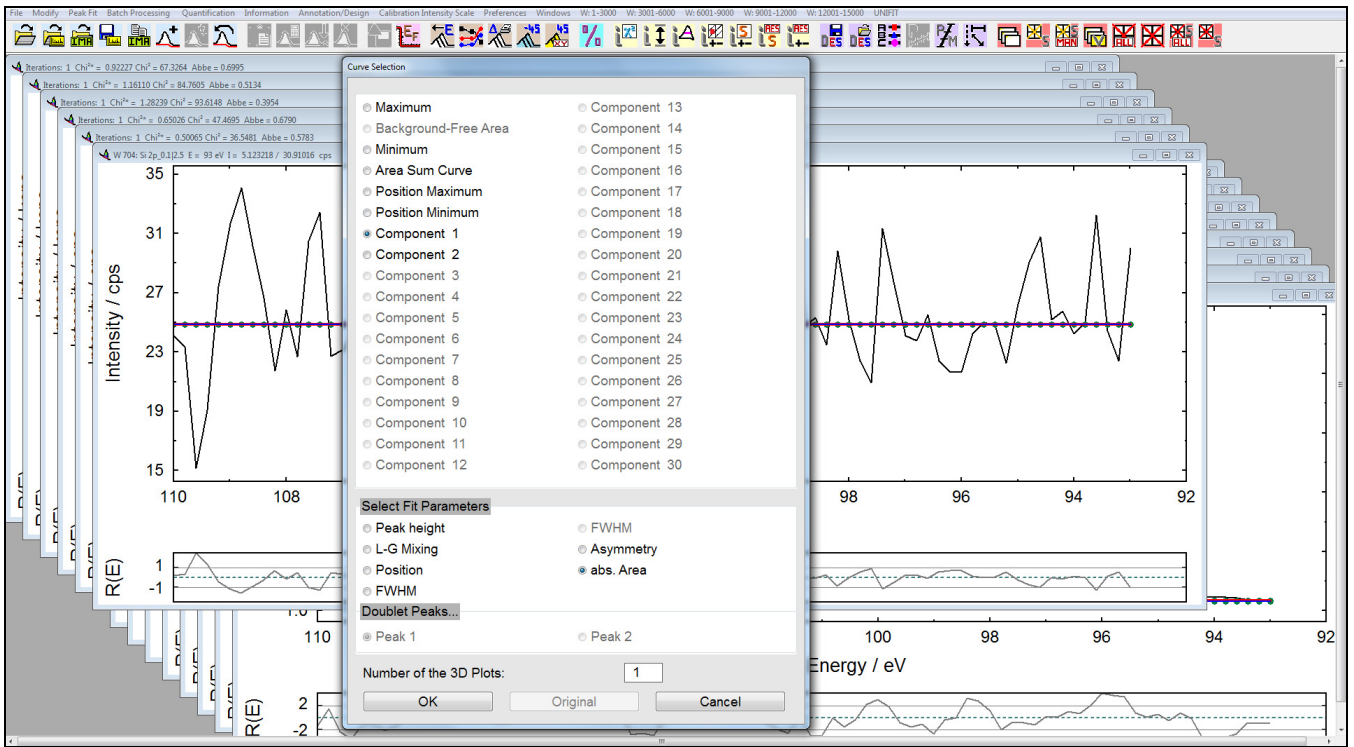


Fig. 5. Screen shot: Curve-selection dialogue for the XY-3D presentations, example: Peak fit of the Si 2p peak (two components) of a XPS multipoint measurement

vii) Three new options for the selection of standard windows were implemented:

- a) All windows with a defined X position,
- b) all windows with a defined Y position,
- c) all windows with the a χ^2 * greater than a defined χ^2 * (after a peak fit).

Additionally, the number of the selected windows is displayed (see Fig. 6).

viii) The loading of images (all typical formats, e.g. *.bmp, *.tif, *.jpg ...) was implemented. If a window with an image is activated, then the processing tools are deactivated. The loaded images can be plotted, exported or saved in a Unifit project.

ix) Now, in some dialogues the changing of the dialogue size is available directly. With the buttons '- DS' and 'DS +' the size can be decreased or increased in one step (see Fig. 1, bottom).

x) In the fit-parameter dialogues the changing of the activated component can be carried out using two new buttons. With the buttons '- AP' and 'AP +' a lower or higher peak-fit component can be activated for the input (see Fig. 1, bottom).

xi) A fourth method was implemented in the new software. Next to photoelectron spectra (XPS), Auger electron spectra (AES) and X-ray absorption spectra (XAS) Unifit 2018 offers the data analysis for RAMAN spectra.

xii) Five new measurement data formats were implemented in the input routine. Now RAMAN spectra with different formats may be loaded. During the input procedure the data are converted to an equidistant step width. The following formats are readable:

- a) S-I VistaControl (*.TVF) (generated by the software S&I VistaControl),

- b) S-I VistaControl XY Multipoint Measurement (*.CSV) (generated by the software S&I VistaControl)
- c) RRUFF (*.TXT) (special RAMAN-input routine for the RRUFF-reference RAMAN spectra),
- d) 1.Column WN increasing/2.Column: Intensity (*.CSV),
- e) 1.Column WN decreasing/2.ColumnIntensity*.CSV).

If the file names have a batch number, a loading of a complete set of files is possible.

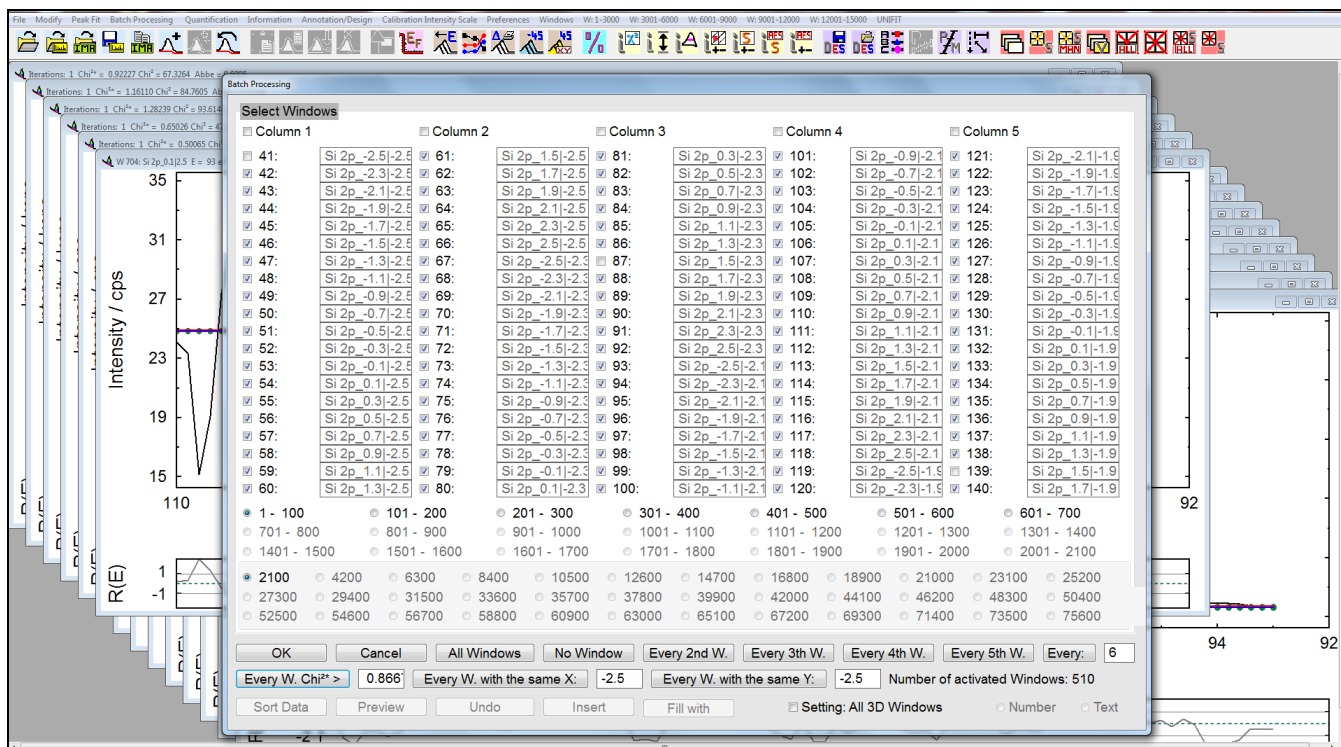


Fig. 6. Screen shot: Standard-window selection dialogue, example: Peak fit of the Si 2p peak (two components) of a XPS multipoint measurement