

TOF-DR Software Release Notes

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Release 3.0.0 – October 2018 (Win7; 32-Bit)

Release 3.0.0 – October 2018 (Win7/Win10; 64-Bit)

1. Introduction

This release includes many new features, including PeakID Review, Auto-PeakID-labels, SlidePreview for PowerPoint, ProfileReview (now part of ImageReview) utility and others.

2. New Features

- a) PeakID Review - PeakID is now a review utility, with the purpose of quickly identifying the peaks that are seen on the current graph in the Spectrum Window.
- b) Auto-PeakID-labels (extends the Auto-AMU-Label capability) now tries to identify each peak automatically with a fragment or permutation label. Note that the AMU tool button is now a 3-way toggle (Auto-AMU labels, Auto-PeakID labels, or No Auto-labels).
- c) Slide Preview with templates for PowerPoint. The new Slide Preview window allows the user to choose a template and preview how the exported slide will look in PowerPoint.
- d) Profile Review is now incorporated into the Image Review Utility -- empowers the user to instantly inspect any profile curve from any peak in the current acquisition, including MSMS data peaks.
- e) Quick Poisson (detector deadtime) intensity correction of a profile curve. In the Profile Window of TOF-DR, select the profile curve(s) of interest in the list view and click Profile|Quick Poisson Correction, and a corrected curve will be added.
- f) The Raw Mass Shift utility has been extended with Z-mode correction. In Z-mode, the acquisition data is divided into time-slices (thickness determined by the Frames Per Slice value) so that a correction factor is calculated for each and every slice (Note that Z-mode does not divide the data laterally into a grid). As a final step you may re-save the corrected raw file, as before.
- g) Now, when the user adds a profile curve during an acquisition, the already-acquired data will be snap-summoned into the curve so that the complete set of datapoints for the entire acquisition thus far will appear in the curve.
- h) When the user adds Peak-ID labels to a spectrum, they will be saved/restored in the .tdc file.
- i) Added the 'Exclude Sub-Threshold Tiles' checkbox to the Raw Mass Shift utility (for XY-mode).
- j) In Image Review, Left/Right arrow keys now shift the bottom axis.
- k) In the Job Wizard, the Total Ion species may now be chosen for evaluation or normalization
- l) In the Job Wizard, a verbose output mode is now supported.

3. Defects Corrected

- a) Resolved a problem with dead time correction, in which an end-of-file stream error occurred.
- b) Now, when loading a .tdc file with an improperly terminated file, the error will be handled.
- c) Now, when the user has 'Max. Expanders' set zero, and adds one (or more) manually, these manually added expanders will not be AutoPlaced by default.
- d) Fixed a problem in the Spectrum Window for MassLinked axes when corral is enlarged / shifted.
- e) Fixed an issue where the MSMS Total Ion profile curve was too low (when acquired over a wide mass range).
- f) Fixed a problem in the Peak Window with the NewPeak button sometimes selects/highlights an existing peak (rather than the NewPeak) for editing.
- g) Fixed a problem with PCA Window .BIF file export when exporting mosaic map data to BIF file.
- h) Fixed a problem with Trace Metals Window, for 64bit addressing, in order to access the TraceMetal Fragment database.
- i) Fixed a problem with calculating mass for a single character chemical abbreviation.
- j) When copying images to clipboard, the comment area color is now uniform – whereas formerly, the selected image had a different color (yellow).
- k) Fixed a problem in PrintPreview where Sigma character 'Σ' was garbled.
- l) Fixed a problem with Image Window overlay panel, to show correct Mosaic Map scaling.
- m) Fixed a problem with saving profile data using the wrong file extension.
- n) Fixed a problem with a retained image from Image Review treated as still acquiring

Release 1.5.0 – October 2017 (Win7; 32-Bit)

Release 2.0.0 – October 2017 (Win7/Win10; 64-Bit)

4. Introduction

This release includes many new features, including native 64-bit executable support, the Image Review Utility, Export to PowerPoint and others.

5. New Features

- m) Native 64bit support -- TOF-DR is now available as a native 64bit application within 64bit versions of MS Windows.
- n) Image Review Utility -- Powerful dedicated utility empowers the user to instantly inspect any ion image from any peak in the current acquisition, including Mosaic Maps and MSMS data. Note that this feature is only available in the 64-bit version of TOF-DR.
- o) Multiple Profile Curves from Multiple ROIs -- Extend the Region of Interest (ROI) approach to profile curves, so that multiple sets of profile curves are built from multiple user-defined ROIs.
- p) Snap-Summon Architecture -- The TOF raw ion data is now automatically restructured for fast access when replayed. Note that this feature is only available in the 64-bit version of TOF-DR.
- q) Factored Y-Axis for Spectral Graphs -- To enhance the presentation of spectra, the spectrum y-axis is 'factored' (divided down by a power of 10) with the corresponding factor indicated in the axis label.
- r) Linked Mass Axes in Spectrum Window -- Allow the user to link the X (mass) axis of multiple graphs in the spectrum window, so that they move together, and also to maximize graph height by hiding x-axis tic labels (on all but the bottom graph).
- s) Export Graphs & Images to PowerPoint -- TOF-DR (via VBA) will Launch PowerPoint Insert a new slide and draw directly to the slide. Aspects include Fonts and point sizes, Margins, Image Rows and Columns, Label Superscripts & Subscripts, Linear Axes & Log Axes, Curve Colors, and more.
- t) 3D Image Export to NESAC/BIO Z-Corrector software -- Support 3D image export to the .BIF6 file format for import to NESAC/BIO (D Graham) Z-Corrector software.
- u) Automatic 3D-Image-Stack Files for ImageJ -- TOF-DR now automatically creates the 3D-Species raw binary image-stack files necessary for the 3d-Image data to be imported into ImageJ. Note that the file is instantly and automatically created (no user-action required) and always available.
- v) Lifted Limit on Mass Calibration Species -- The user may now define any number of mass calibration species for calibration refinement. Note that this change to the .tdc and .cal file formats is backwards compatible.
- w) In the Graph-Presentation dialog under Tools|Options, the InitialMassRange properties have been added, which determine the initial mass range in various windows and forms for spectral graphs.
- x) Allow user to modify the linescan averaging width from a right-click popup menu on the linescan viewer in the image window.
- y) Export to ASCII for image data. Choose the File|SaveAs menu option in the Image Window, which now provides the "ASCII portable gray map file (*.pgm)" filetype.
- z) The "Spectrum Save-As ASCII unit mass .Asc" option now supports an extended mass binning feature. The new dialog for ExportAsTextMassBinned allows the user to specify the BinSize, MassRange etc.
- aa) Extended the playback UI time window limit feature so that the user may optionally define a cycle range window.

6. Defects Corrected

- o) Save subtracted spectra to .tdc file now saves properly.
- p) The Image Inspector Cursor Info now updates properly on the right side in the cursor area.
- q) TOF-DR will now choose a more appropriate mosaic map resolution value for a Mosaic Map Live-Acquisition. TOF-DR will, as a starting point, begin with mosaic map display resolution value designated in SmartSoft-TOF (in the Mosaic tab of the Acquisition properties form), and will automatically enlarge this value if it is too small.
- r) In the ROI Editor, ensure that a ROI previously defined via sliders (counts subrange) appears 'as before' when advancing from one ROI to another within a session.
- s) Correct the lingering 'Acquiring' label that appears in the Spectrum Window form caption (title) --or in the application title bar if the spectrum MDI window is maximized -- after an acquisition is complete.

I. TOF-DR Image Review Utility Release Notes

In Version 2.0 64-bit only

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Image Review Utility Overview

The Image Review Utility is a dedicated window that allows the user to quickly step from peak to peak and instantly inspect any corresponding ion image from the current acquisition (or most recently replayed raw file).

To launch the Image Review Utility from 64bit TOF-DR, first replay a raw file, then choose the “Tools | Image Review Utility” menu option, or else click on the Review button in the main toolbar, as shown in the figure below.

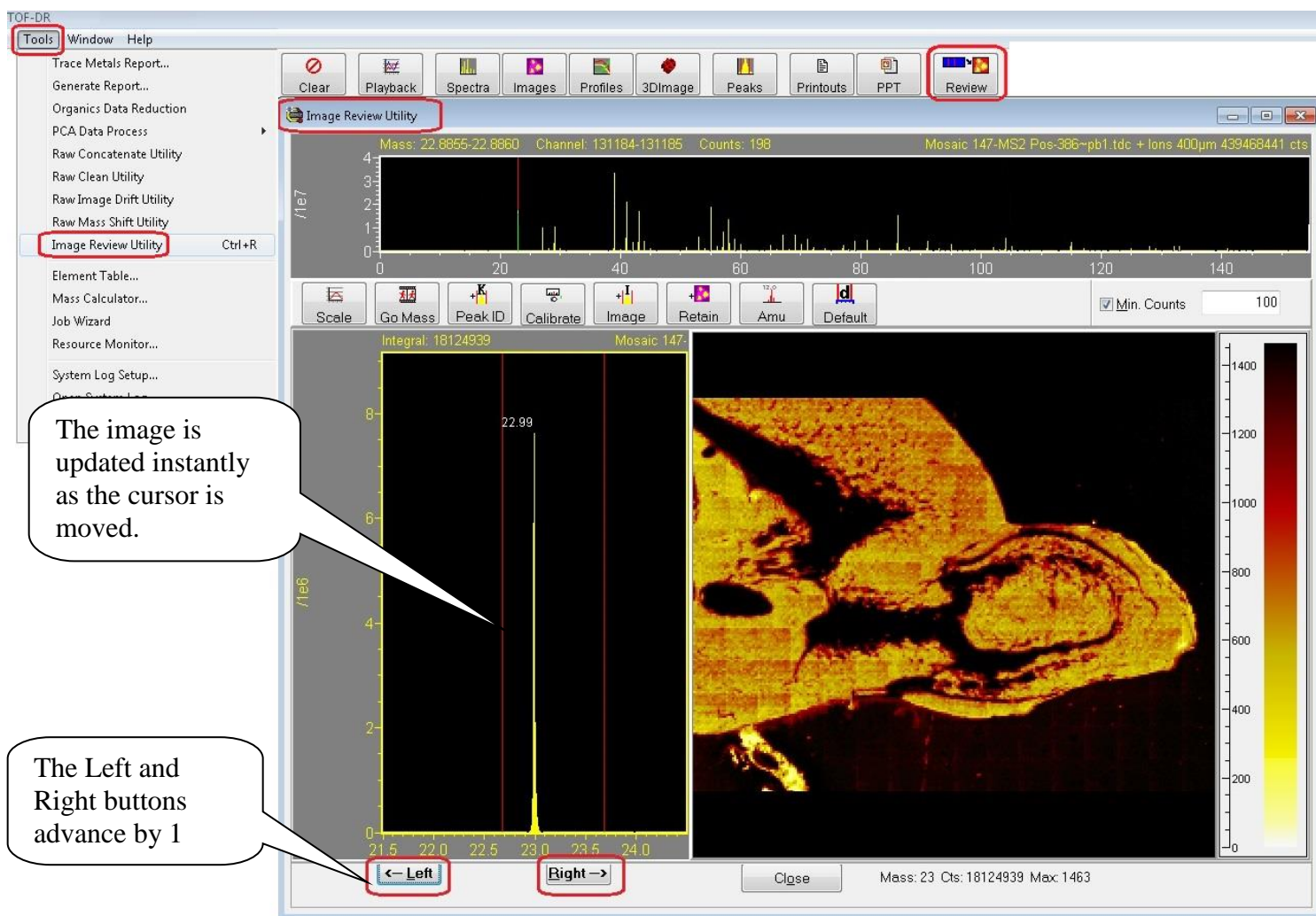


Figure 1 –The image Review Utility

Adjust the spectrum cursors and the corresponding image will appear instantly. Or, click the Left or Right buttons as shown to advance by 1 amu and instantly update the corresponding image.

Note that this feature supports normal ion images, mosaic map images, and both normal and MSMS data.

Note that this feature is only available in the 64-bit version of TOF-DR. This feature takes advantage of 64bit addressing for highly optimized image retrieval speed.

Tools in the Image Review Utility

A number of tools are available in the ImageReview Utility that also appear in the Spectrum Window toolbar and function in the same way:

- Scale – Auto-scale the spectrum graphs and the image color bar
- Go Mass – Jump to any mass or species
- Peak-ID – Identify a species and optionally drop a label
- Calibrate – Mass calibrate the spectrum
- Image – Define an imaging peak in the Peak Window for future acquisitions
- Amu – Show/Hide amu labels on the spectra

In addition, there are a number of new tools available:

- Retain – Send the current image to the Image Window (i.e. it will be added to the list in the Image Window, where it can be saved/manipulated in the normal manner)
- Default – Restores the double cursor delta range and x-axis delta range to default values
- Min. Counts – A threshold value and a checkbox, which when checked will cause the Left/Right (shift x-axis) buttons to skip peaks below this threshold

Image Review Utility during a Live Acquisition

The Image Review Utility may be used in the normal way during and after a live acquisition.

Also note that whenever a new imaging peak is defined in the PeakWindow during a live acquisition, the previously acquired data for that ion image will be included automatically, so that the full ion image for the entire acquisition will be displayed and continue acquiring in the usual manner.

Optimization of Raw File Data

In order to implement the Image Review Utility, whenever a raw data file is processed (whether as part of a live acquisition or raw file replay), the data is optimized and retained so that subsequently the user may rapidly summon an image from this data set at any time until another raw file is processed.

This optimized raw data is currently saved as a set of temporary files in a dedicated folder on the hard disk. Therefore, this feature requires the availability of free disk space and the size of this disk space is approximately the same (somewhat smaller) than the original raw file being replayed.

Note that if free disk space available is below a threshold, then this feature will automatically be disabled.

II. TOF-DR Snap-Summon of Images – Release Notes

In Version 2.0 64-bit only

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- 5 Future Extensions of Snap-Summon **Error! Bookmark not defined.**

Snap-Summon of Images Overview

Snap-Summon allows the user to quickly inspect any ion image from the current acquisition (or most recently replayed raw file). The user positions a double cursor around any peak in the spectrum, and 'summons' a corresponding image, which is immediately displayed in the image window.

Note that this feature is only available in the 64-bit version of TOF-DR.

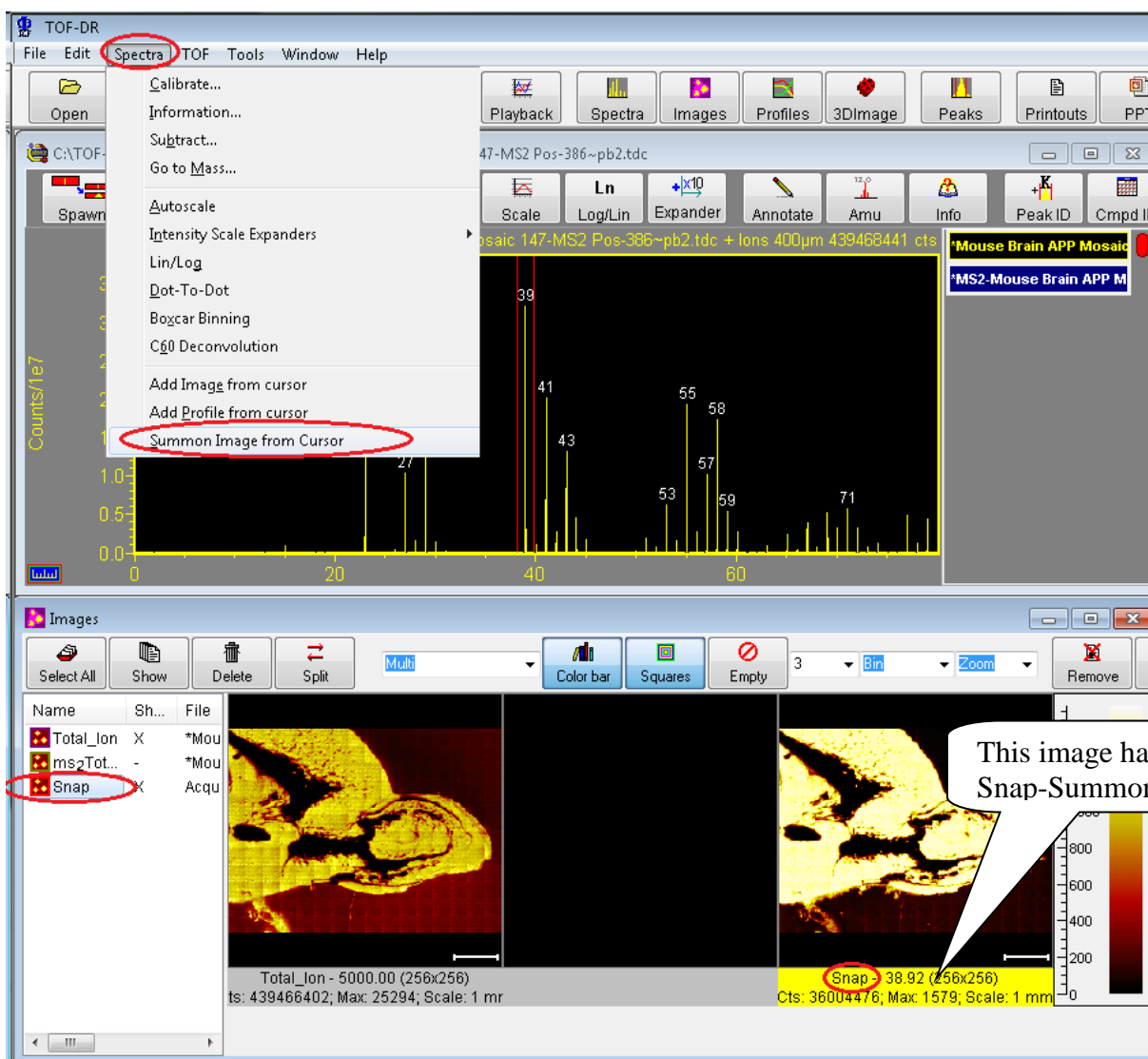


Figure 1 – An ion image has been ‘Snap-Summoned’ to appear in the Image Window.

In the figure above, a spectrum and total-ion image from a mosaic map acquisition is shown, and note that playback of this multiple-gigabyte raw file required several minutes to complete. Subsequently, the double cursor was positioned around the peak at mass 39, and via the menu option indicated, a new ‘Snap-Summoned’ image was built and displayed in the Image Window within several seconds.

Note that this feature supports normal ion images, mosaic map images, and both normal and MSMS data.

The user may snap-summon another image as often as desired, and in this way rapidly inspect multiple ion images suspected to be of interest. Note that when a new image is snap-summoned, any prior image data in the Snap-Image will be replaced by the new image data by default.

Retaining a Snap-Summoned Image

When the user encounters a snap-summoned ion image of interest, the snap-image can be retained as shown in the figure below.

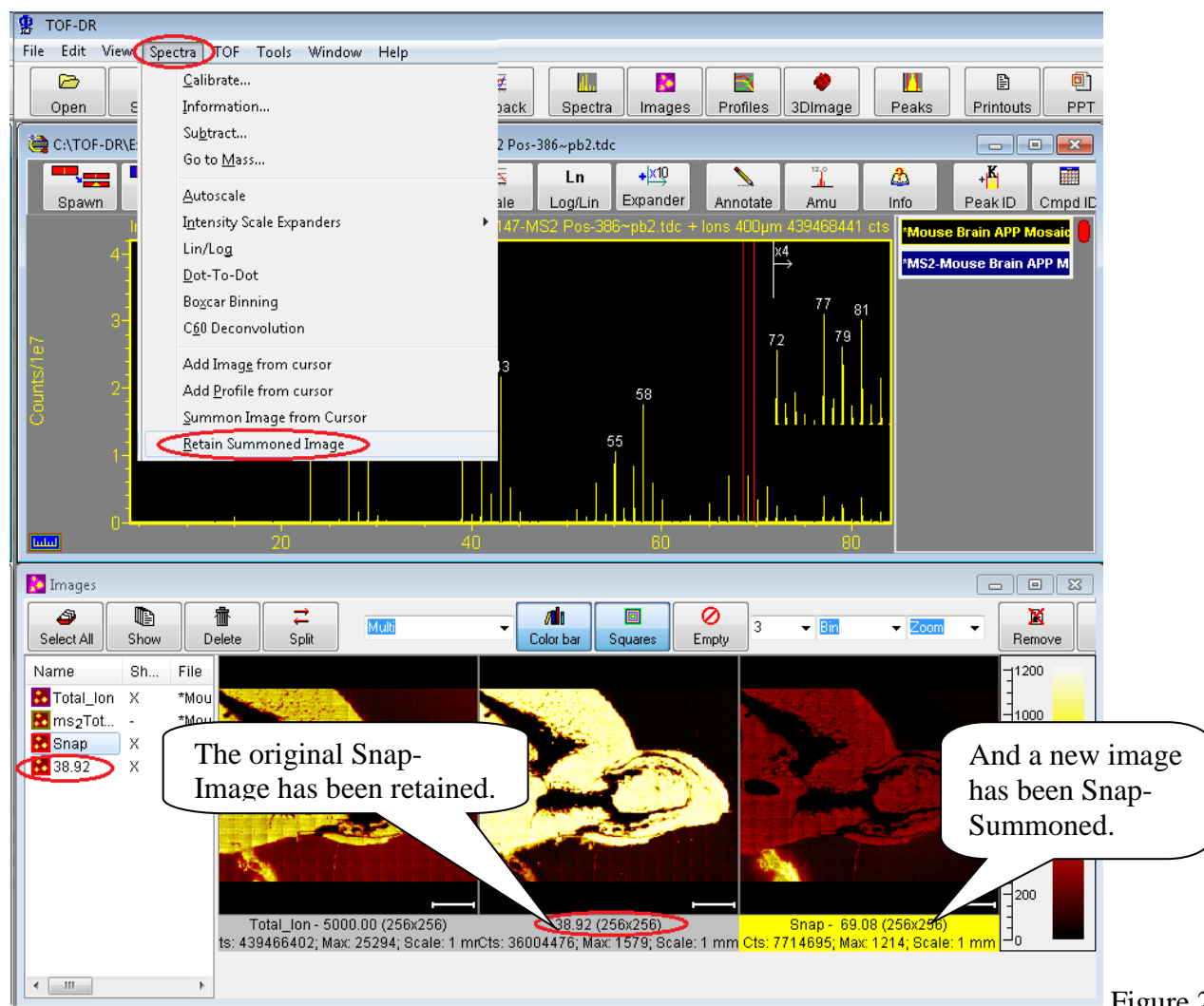


Figure 2

– The original Snap-Image has been retained.

In the figure above, the original Snap-Image has been retained, and this retained ion image can be examined or saved for future reference in the same way as any other image.

Snap-Summon during a Live Acquisition

The Snap-Summon feature may be used in the normal way during and after a live acquisition.

Additionally, whenever a new imaging peak is defined in the PeakWindow during a live acquisition, the previously acquired data for that ion image will be snap-summoned automatically, so that the full ion image for the entire acquisition will be displayed and continue acquiring in the usual manner as shown in the figure below.

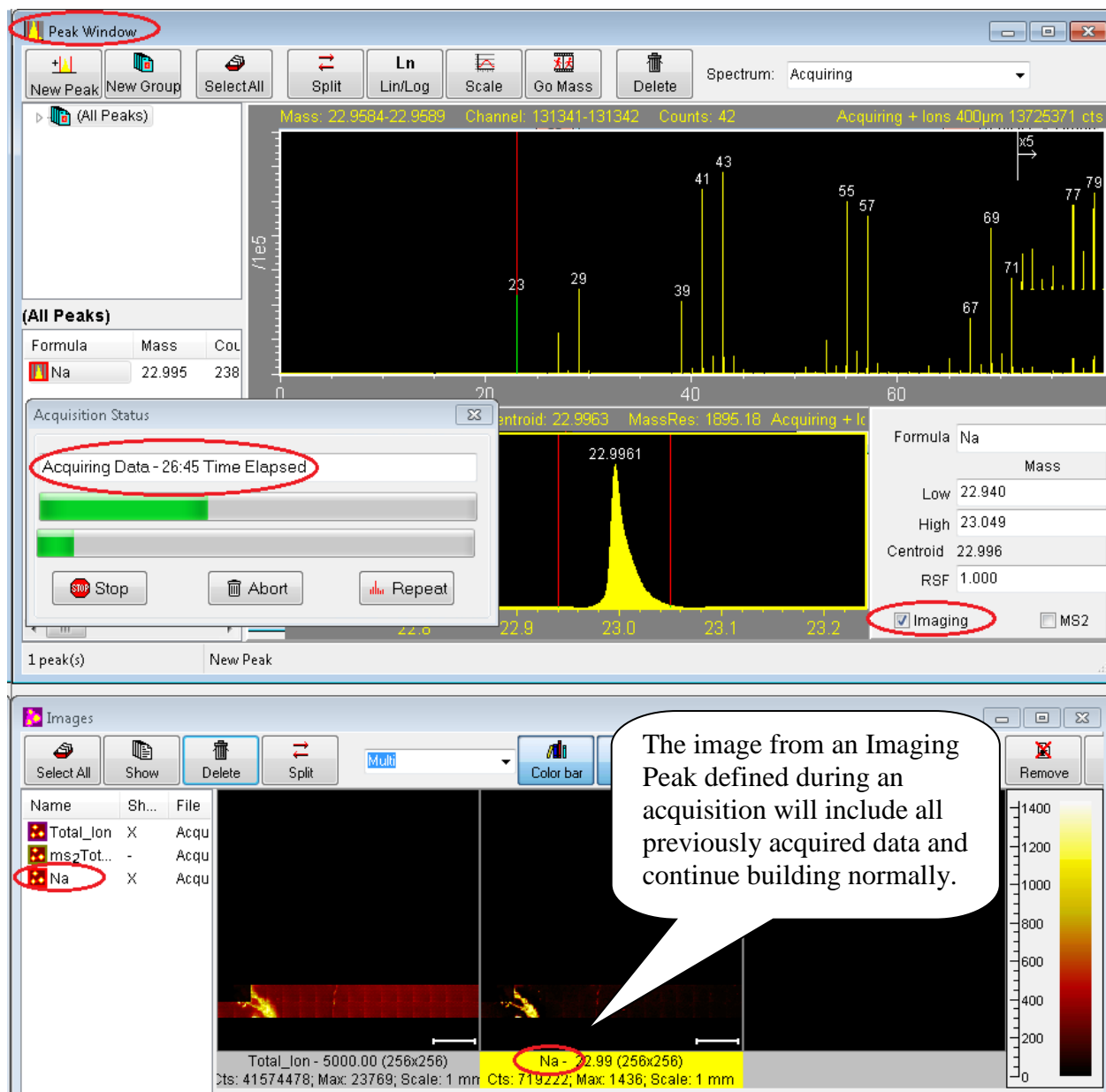


Figure 3 – The image from an Imaging Peak defined mid-acquisition will show all previously acquired data.

Optimization of Raw File Data for Snap-Summon

In order to implement the Snap-Summon feature, whenever a raw data file is processed (whether as part of a live acquisition or raw file replay), the data is optimized and retained so that subsequently the user may rapidly summon an image from this data set at any time until another raw file is processed.

This optimized raw data is currently saved as a set of temporary files in a dedicated folder on the hard disk. Therefore, this feature requires the availability of free disk space and the size of this disk space is approximately the same (somewhat smaller) than the original raw file being replayed.

Note that if free disk space available is below a threshold, then this feature will automatically be disabled.

This feature takes advantage of 64bit addressing in TOF-DR for highly optimized image retrieval speed.

III. Export Graphs & Images to PowerPoint Release Notes

TOF-DR Version 1.5/2.0

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Export Graphs & Images to PowerPoint Overview

The Export Graphs & Images to PowerPoint feature allows TOF-DR to send the graphs/images from the current window directly to PowerPoint as a new slide and using the margins and font sizes specified by the user. This capability may be invoked from the Spectrum Window, the Image Window or the Profile Window.

Spectrum Window

In order to export the spectra currently visible in the Spectrum Window, Choose the Edit | Copy to PowerPoint menu option as shown below.

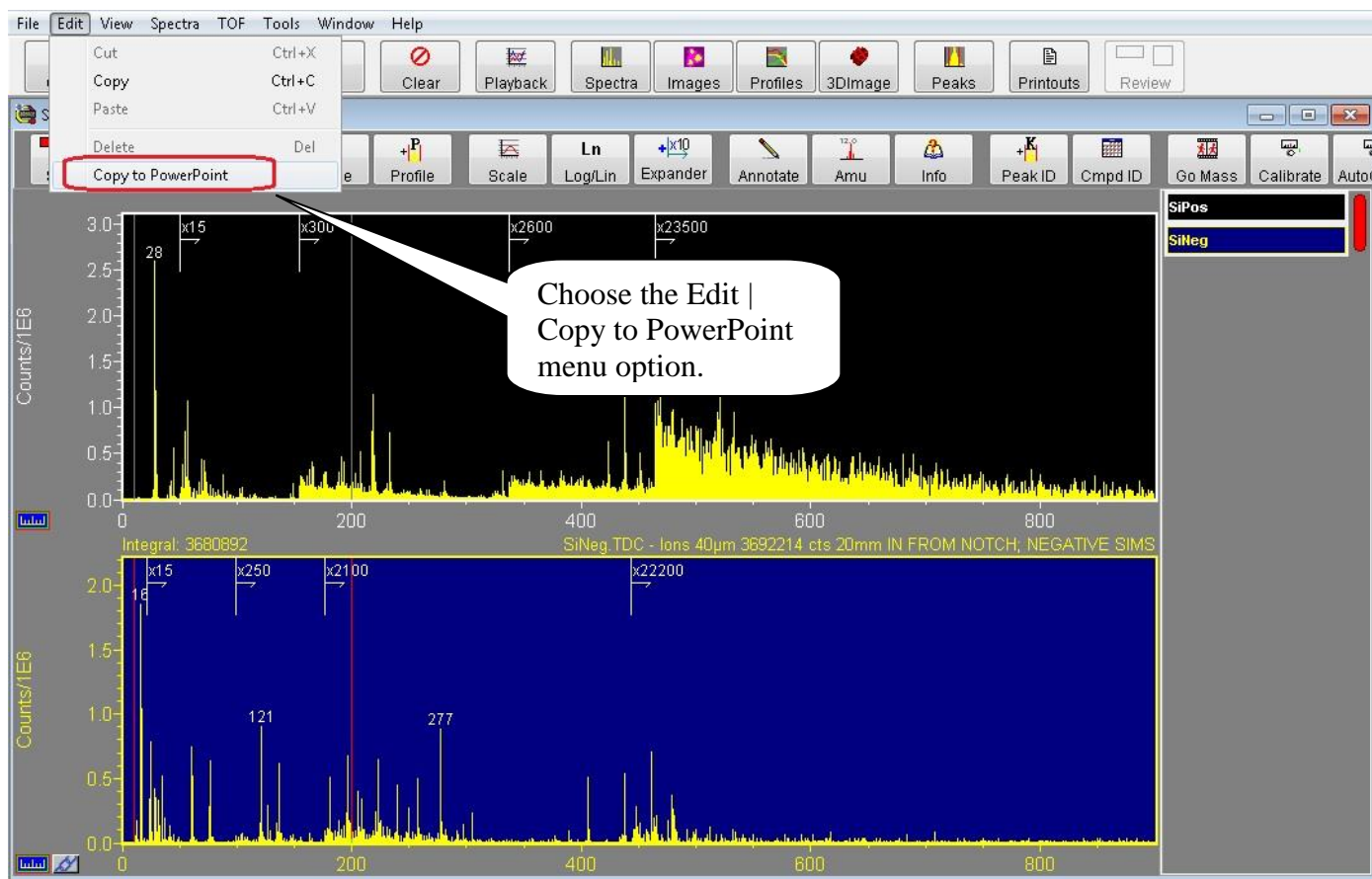


Figure 1 – Spectrum Window Edit | Copy to PowerPoint menu option

The Export to PowerPoint dialog will appear as shown below

The screenshot shows the 'Export to PowerPoint' dialog box. It has a title bar with standard window controls. The 'Settings' section at the top includes a dropdown menu set to 'PREVIOUS' and four buttons: 'Load', 'Save', 'Delete', and 'File...'. Below this is the 'Margins' section, which specifies a density of '(72 points/in – 28.3 points/cm)' and contains four input fields for 'Top (points)', 'Bottom (points)', 'Left (points)', and 'Right (points)', all set to '72'. The 'Font' section shows 'Arial' as the selected font with a 'Choose Font' button. The 'Font Sizes' section contains four input fields: 'Axis Tic Label (points)' set to '10', 'Axis Label (points)' set to '11', 'Information Line (points)' set to '8', and 'Labels (points)' set to '8'. At the bottom, there is a checked checkbox for 'Append Slide at Bottom' and an 'Export to PPT' button. Two callout boxes are present: one on the left pointing to the 'Information Line (points)' field with the text 'Note that the Information Line Font Size can be set to 0 in order to hide the corresponding text box.', and one on the right pointing to the 'Export to PPT' button with the text 'When all values on the form are set properly, click the ‘Export to PPT’ button.'

Figure 2 – The Export to PowerPoint dialog

Specify the Margins (in points), the Font, and the Font Sizes (in points) in the dialog.

Note that the Information Line Font Size can be set to 0 in order to hide the corresponding text box on the slide (and this also creates a bit more space for the graphs).

If the 'Append Slide at Bottom' checkbox is checked, then the new slide will be created at the bottom of the current PowerPoint presentation, otherwise the new slide will be inserted at the current position within the presentation.

Note that this set of settings (Margins, Font & Font Sizes etc.) may be saved and reloaded in the future by specifying a Settings Name and clicking the Save or Load button as appropriate.

When all values on the form are set properly, click the 'Export to PPT' button.

Now, TOF-DR will launch the PowerPoint program (if necessary), create the new slide, and draw the graph(s) and curve(s) directly on the slide as shown below.

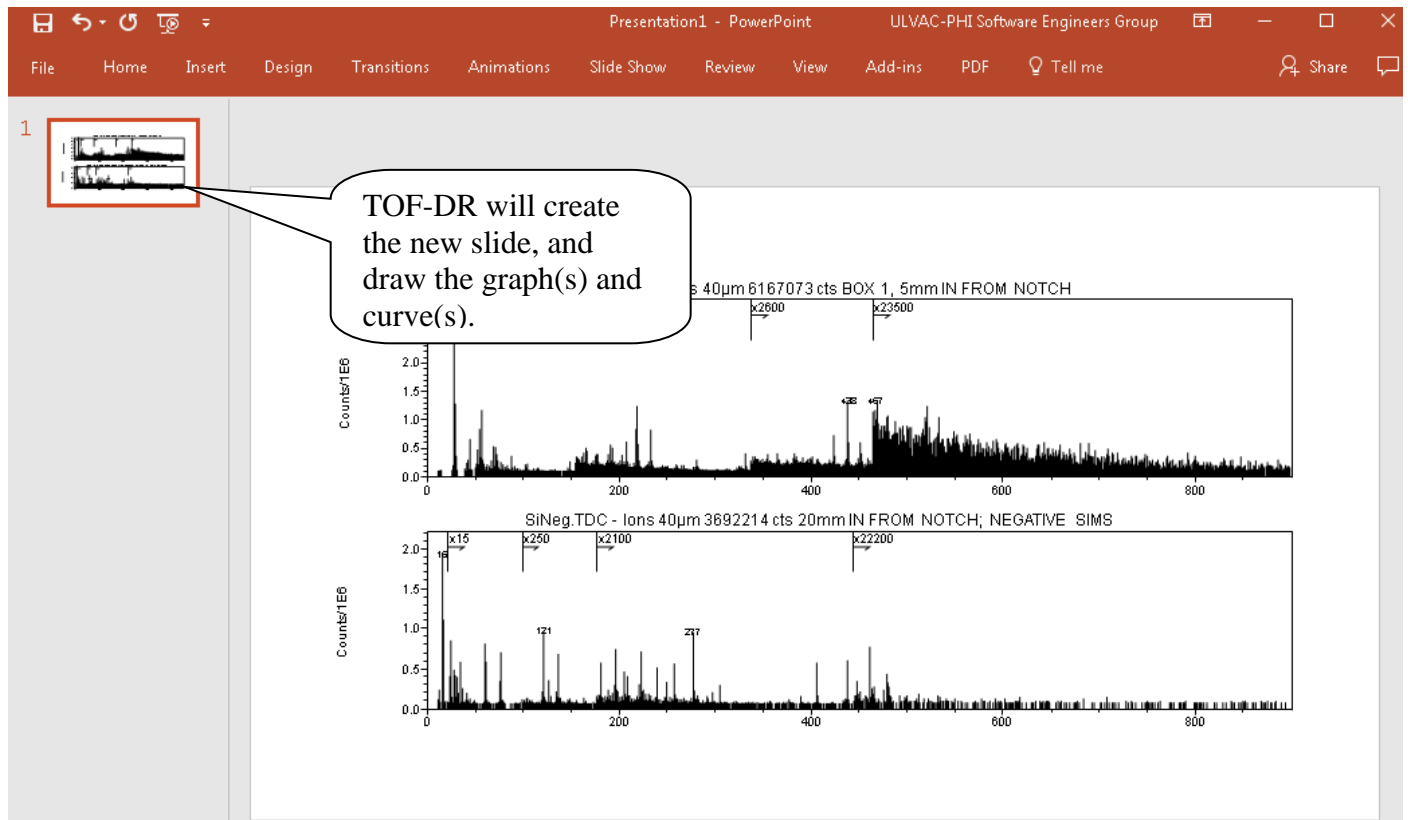


Figure 3 – The Newly Created Slide in PowerPoint

Profile Window

In the Profile Window, in order to export the graph and profile curves currently visible, choose the Edit | Copy To PowerPoint menu option as shown in the figure below.

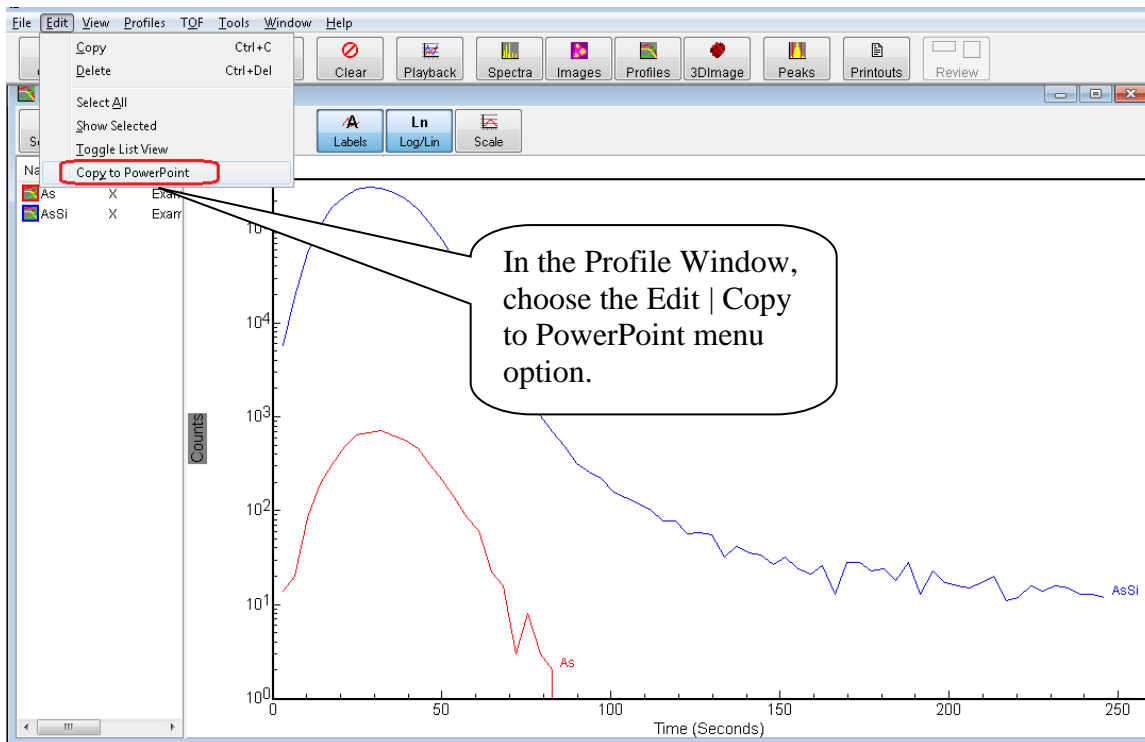


Figure 4 – Profile Window Edit | Copy to PowerPoint menu option

Follow the process as described above (i.e. when all values on the Export to PowerPoint dialog are set properly, click the 'Export to PPT' button), and TOF-DR will create the new slide, and draw the graph and curves directly on the slide as shown below.

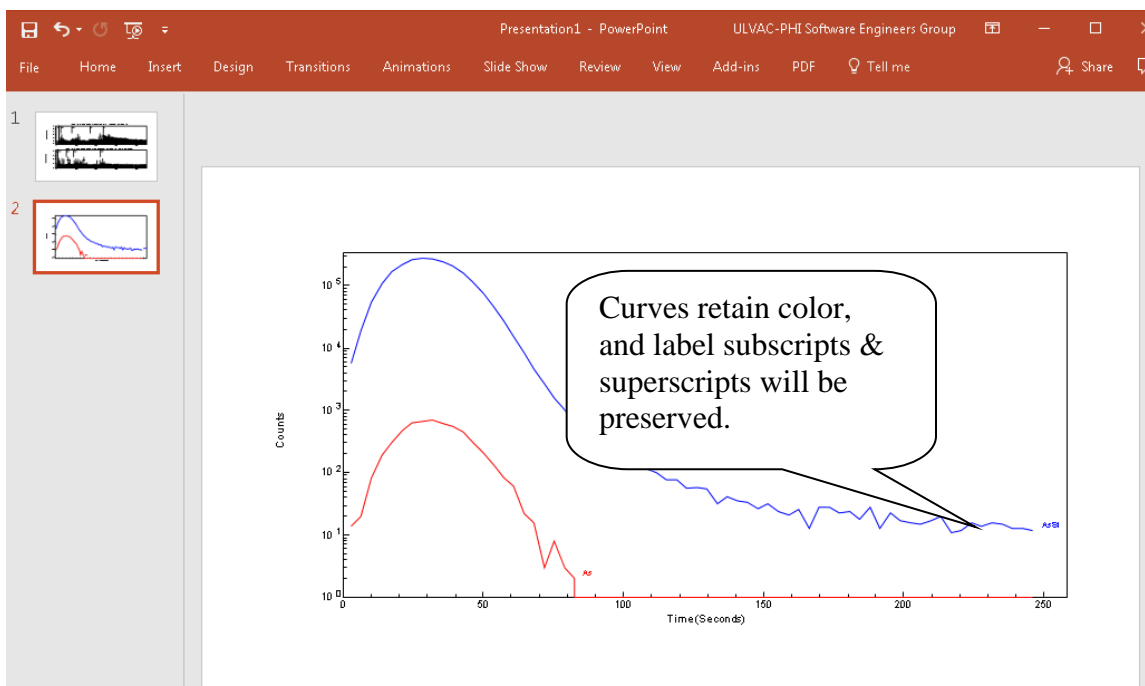


Figure 5 – The Newly Created Slide in PowerPoint

And note that curves should retain their color, and subscripts and superscripts for the profile curve labels will be preserved, as expected.

Image Window

In order to export the images currently visible in the Image Window, Choose the Edit | Copy To PowerPoint menu option as shown below.

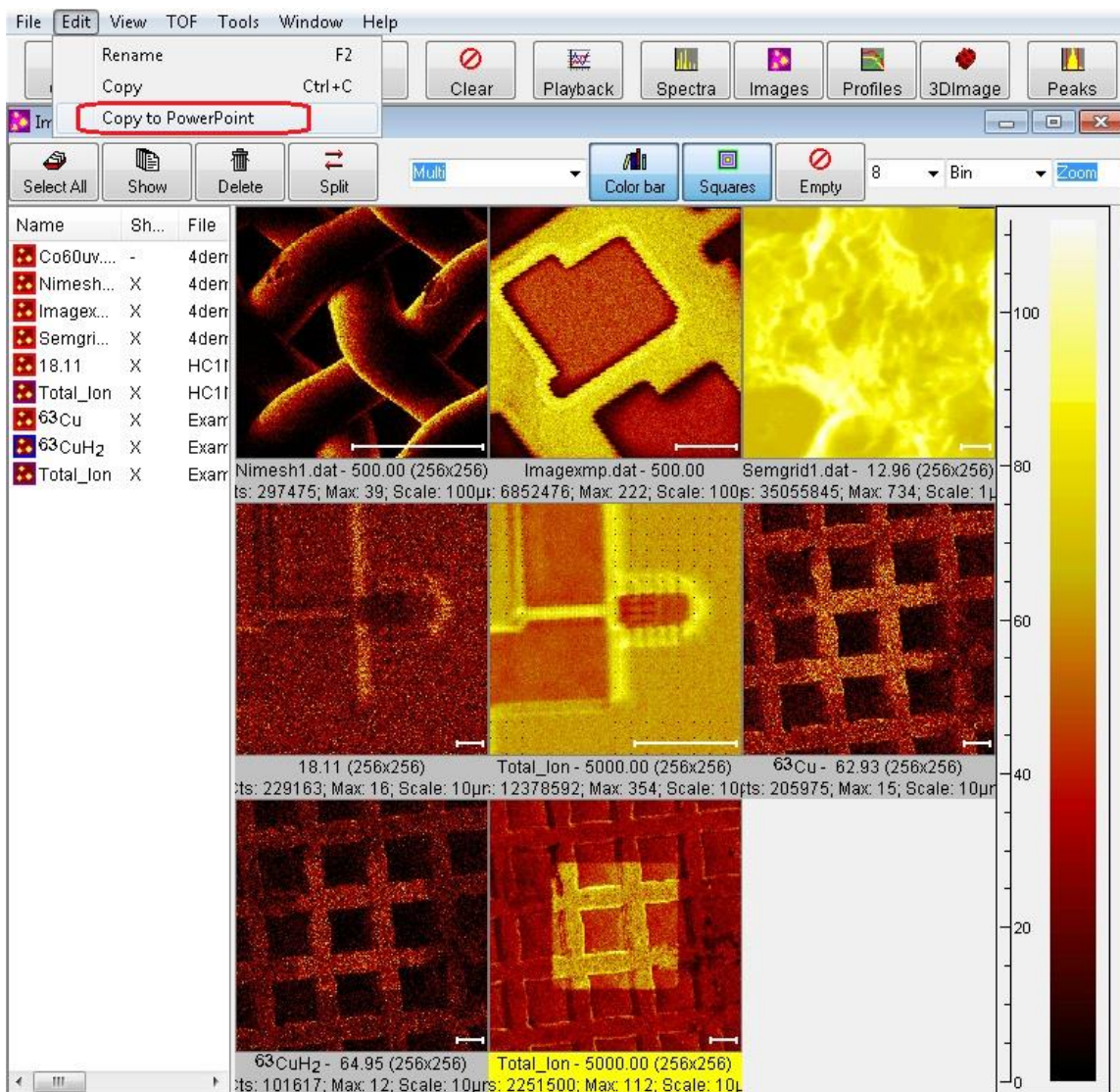


Figure 6 – Image Window Edit | Copy to PowerPoint menu option

The Export to PowerPoint dialog will appear as shown below.

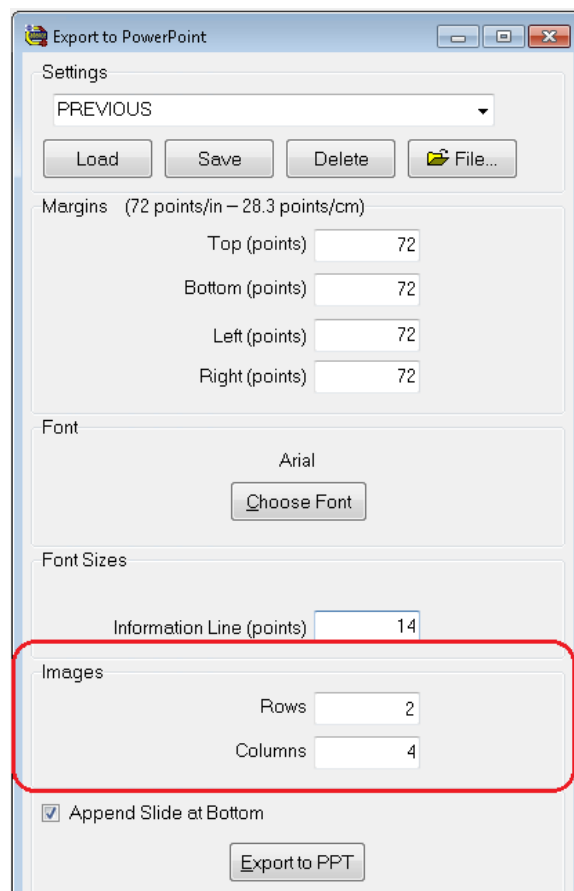


Figure 7 – The Export to PowerPoint dialog with Image Rows and Columns

In addition to the settings described above, choose the desired number of Rows and Columns in which to display the set of images. Note that the rows and columns can be different than that displayed in the TOF-DR Image Window. Also Note that the Information Line Font Size can be set to 0 in order to hide the corresponding text box on the slide (and this may help to create a bit more space for the images).

TOF-DR will create the new slide, and draw the images in the grid pattern as shown below.

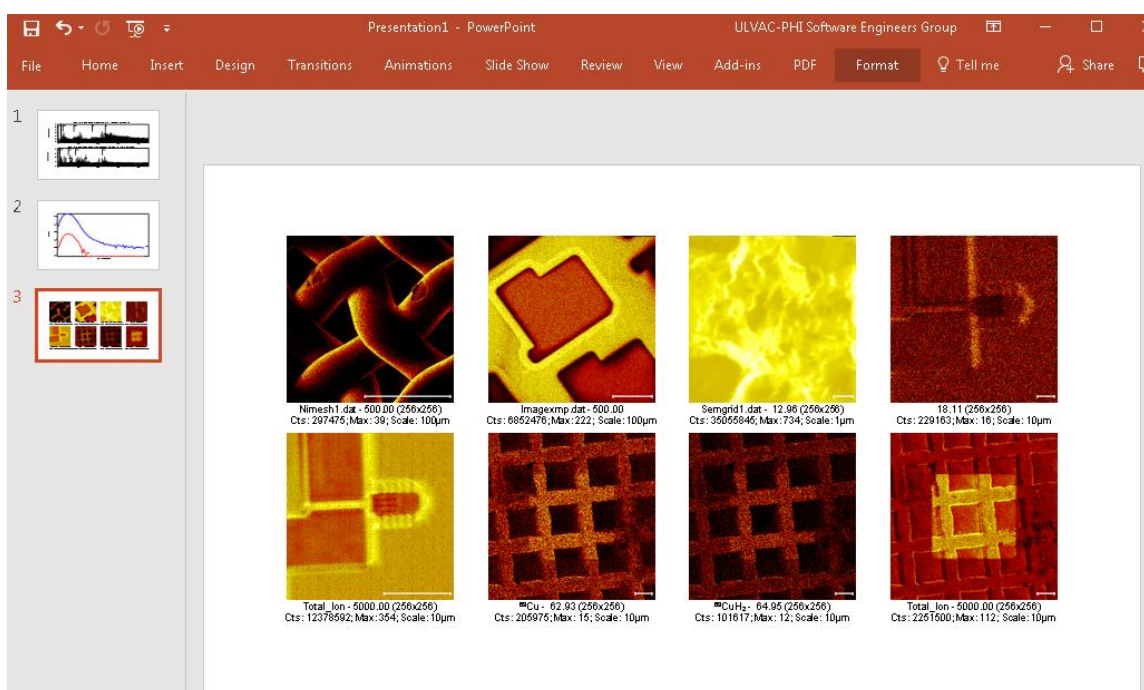
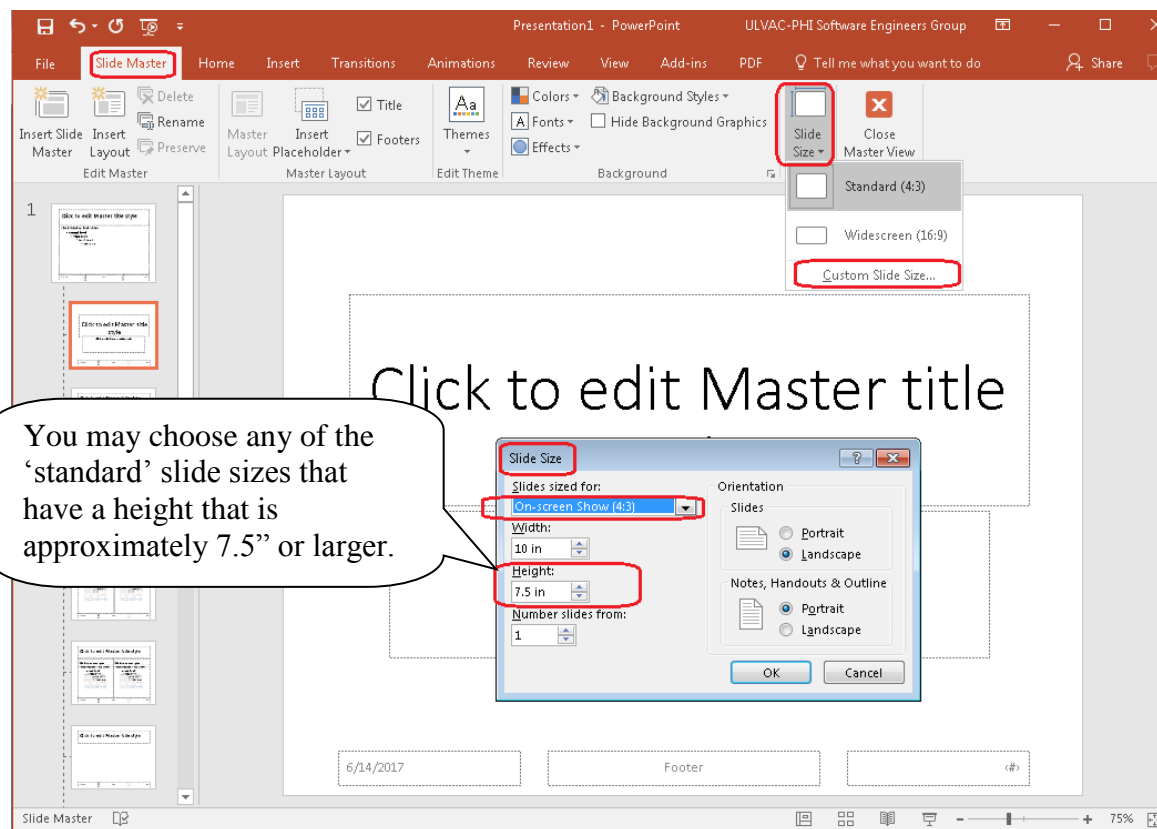


Figure 8 – The Newly Created Slide in PowerPoint

Important Note – Master Slide Height in PowerPoint

In order for TOF-DR to draw properly to PowerPoint, the Master Slide Height for the presentation should be above a minimum threshold of approximately 7.5” or larger. Most of the standard slide sizes provided by PowerPoint meet or exceed this minimum height. However, it is recommended to check this value and correct it if necessary by choosing a different standard size (such as ‘Standard (4:3) or WideScreen (16:9) or A3 Paper or Letter Paper etc.) that meet or exceed this minimum. See the figure below.



IV. Mass Link Axes in Spectrum Window -- Release Notes

TOF-DR Version 1.5/2.0

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Introduction

The Mass Link feature allows the user to 'link' the X (mass) axis of multiple graphs in the spectrum window so that only the tic labels of the bottom axis will be visible, and so that the mass axes will move together when stretched or dragged with the mouse.

Link the Mass Axes

To link the mass axes of the graphs shown in the Spectrum Window, click the Mass Link button that appears in the lower left corner of the graph as shown in the figure below.

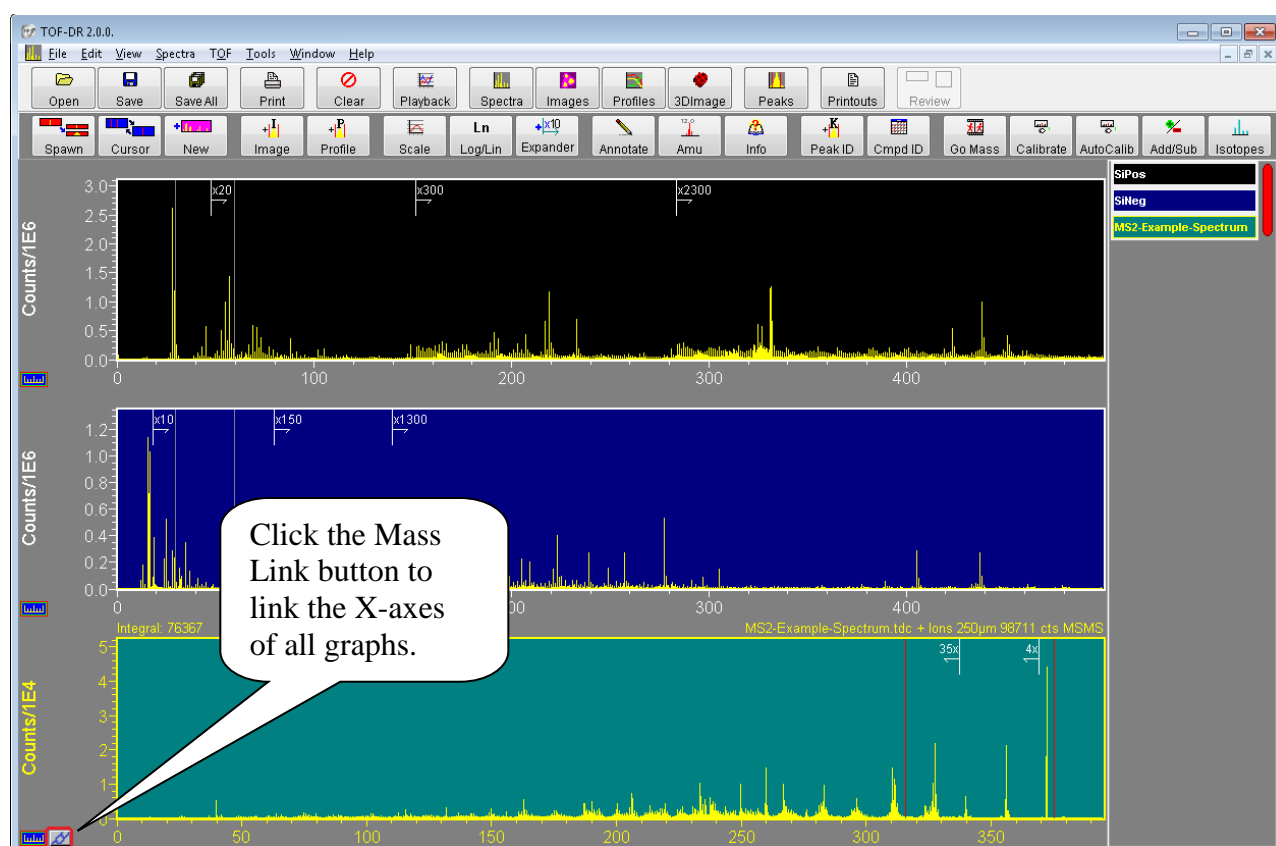


Figure 1 – Click the Mass Link button to link the X-axes

Note that this button will appear when it is possible to link the mass axes – i.e. whenever multiple unspawned-only views are visible together. Also note that only unspawned views are Mass Linkable, and only when no spawned-views are visible. (The reason for this is that the mass axis of the daughter spectrum takes on a sub-range of the mass axis of the parent according to its double-cursor, and so to Mass Link would sever this relationship.)

Now the graphs will be linked as shown below.

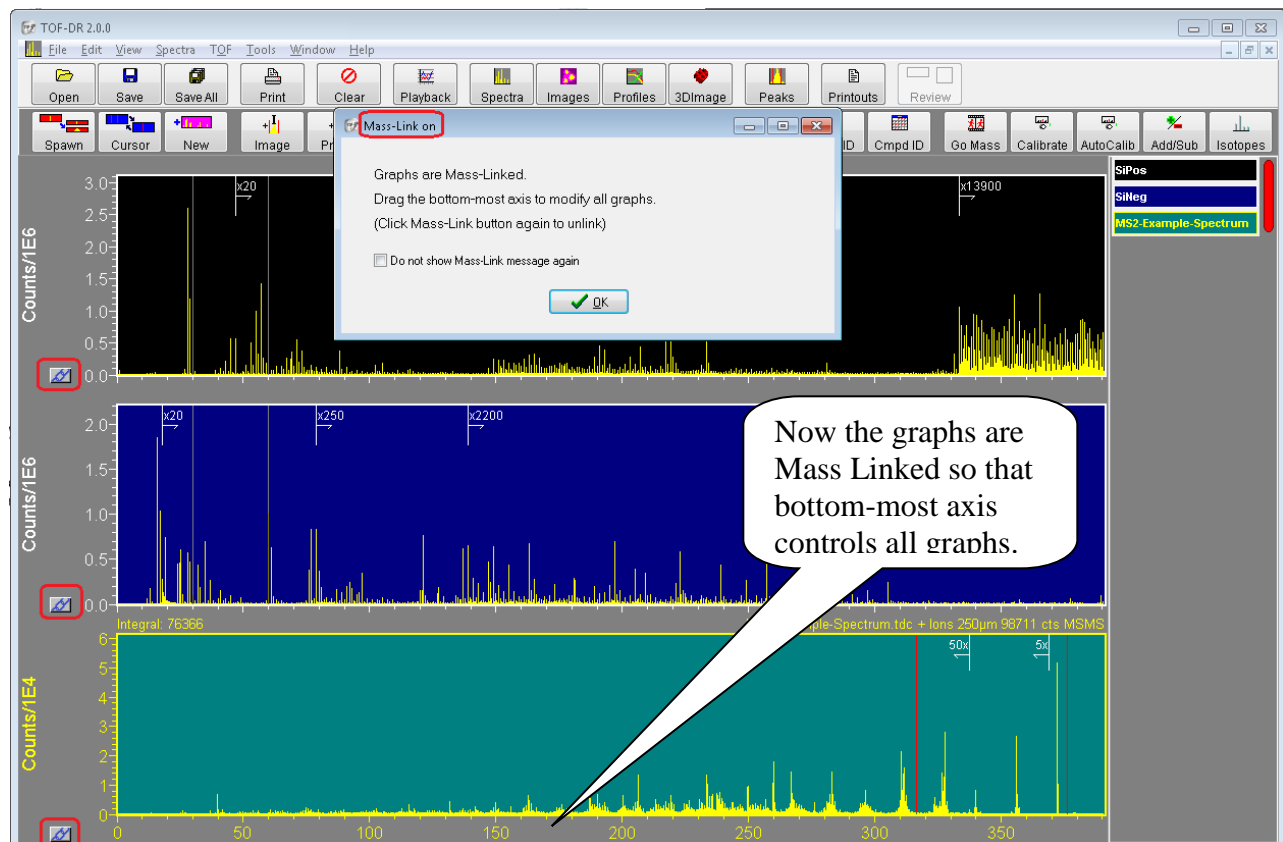


Figure 2 – The Graphs are Mass Linked

Unlink the Mass Axes

To unlink the mass axes, click the Mass Link button (which now appears at the lower left corner of each graph) again. Then all axes will become visible and independent once more.

1. Overview

TOF-DR V1.4.0:

Intensity Scale Expansion Markers on spectra may be placed manually and/or automatically;
Peak-Groups enable the signal from several related ion species to be summed together into a single image, or profile-curve, or 3D-image.

Improvements to spectrum handling and the “Corral”

2. New Features

General

1. Intensity Scale Expansion Markers on spectra. See the Intensity Scale Expansion Markers in TOF-DR – Release Notes below.
2. Peak-Groups support. See the Peak-Groups in TOF-DR – Release Notes below.
3. Improvements to the Spectrum “Corral” for showing the spectrum name, showing the full name as hint via mouse hover. Also, the user may click on the spectrum name in the corral and the view will reposition in order to show the corresponding graph.
4. Support for managing large numbers of spectra in the Spectrum Window:
 - a) Remove the lowest priority set of daughters (but not base) when a new spectrum is added and a user-definable threshold is surpassed.
 - b) Remove the lowest priority spectrum (& any daughter views) when a new spectrum is added and a user-definable threshold is surpassed.

MS2 Support

5. Spectrum SaveAs supports save MSMS NIST format .MSP unit-mass ASCII file type.
6. Replay of MS2 Raw data using ROIs support.

3. Bug Fixes

7. ROI-Editor: The shapes drawing (polygon etc.) line is easier to see.
8. Improvements to how profile data is pasted/ungrouped into PowerPoint
9. Improvements to Copy-Page button in Printout Editor

VI. Intensity Scale Expansion Markers in TOF-DR – Release Notes

TOF-DR Version 1.4

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1. Intensity Scale Expansion Markers Overview

Intensity Scale Expansion Markers -- or 'Expanders' for short -- appear on TOF Spectrum graphs. They indicate that spectrum data beyond (i.e. rightward of) the marker's x-axis position has been multiplied by a factor, e.g. '**x25**' so that smaller peaks at higher mass are visually magnified and not 'lost among the tall trees'.

Compare an example spectrum with and without Expanders as shown below.

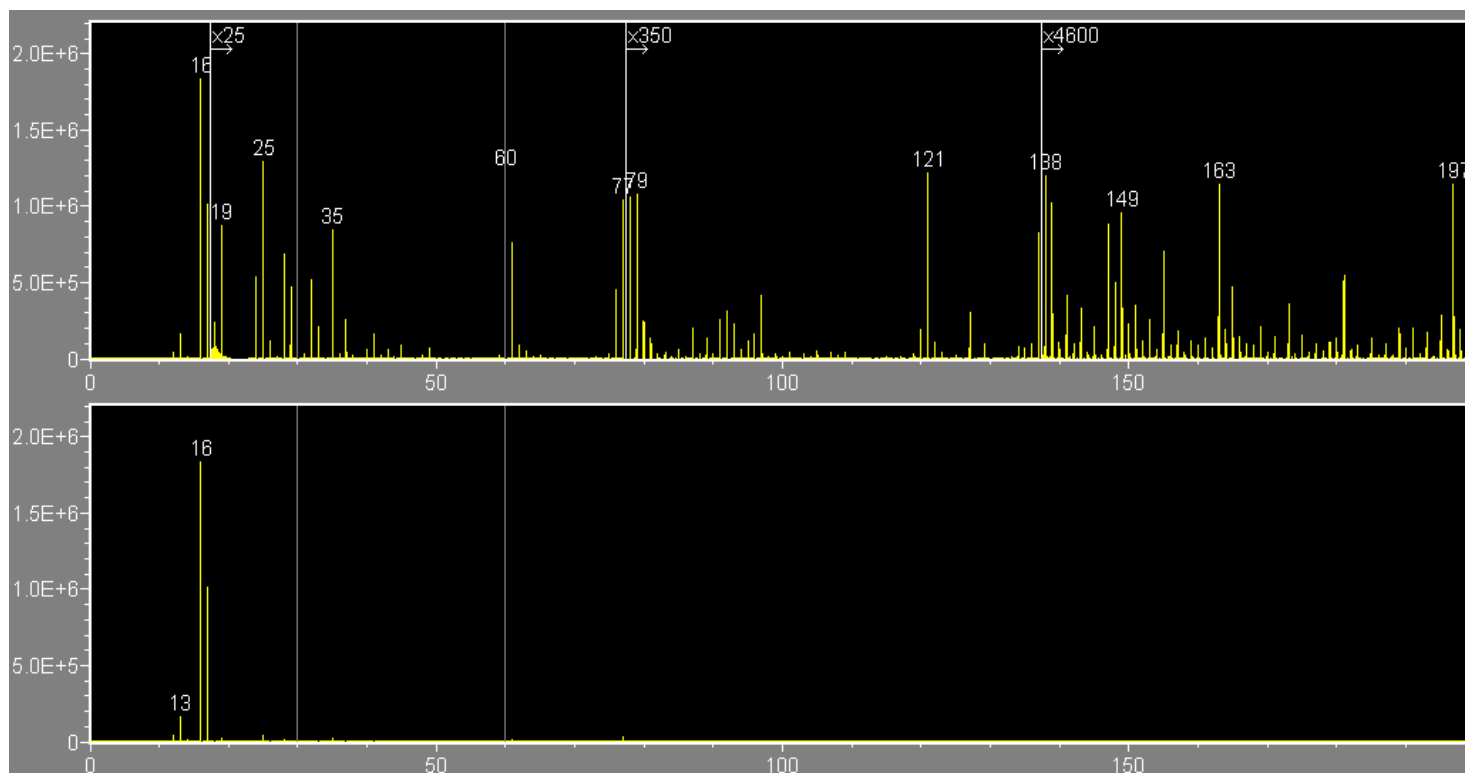


Figure 1 – Spectrum displayed with and without Expanders.

As can be seen in the upper graph, many peaks of interest become apparent that are essentially invisible on a normal linear scale over this mass range.

As will be described below, Expanders may be applied:

- Automatically as part of the normal AutoScale mechanism
- Manually in order to highlight particular features, or in preparation for presentations

2. Applying Expanders Manually

To add a new Expander to the current graph, click on the “Add Expander” tool button in the Spectrum Window toolbar.

To modify an existing Expander, right click on the Expander label to modify it via the context menu as shown in the figure below.

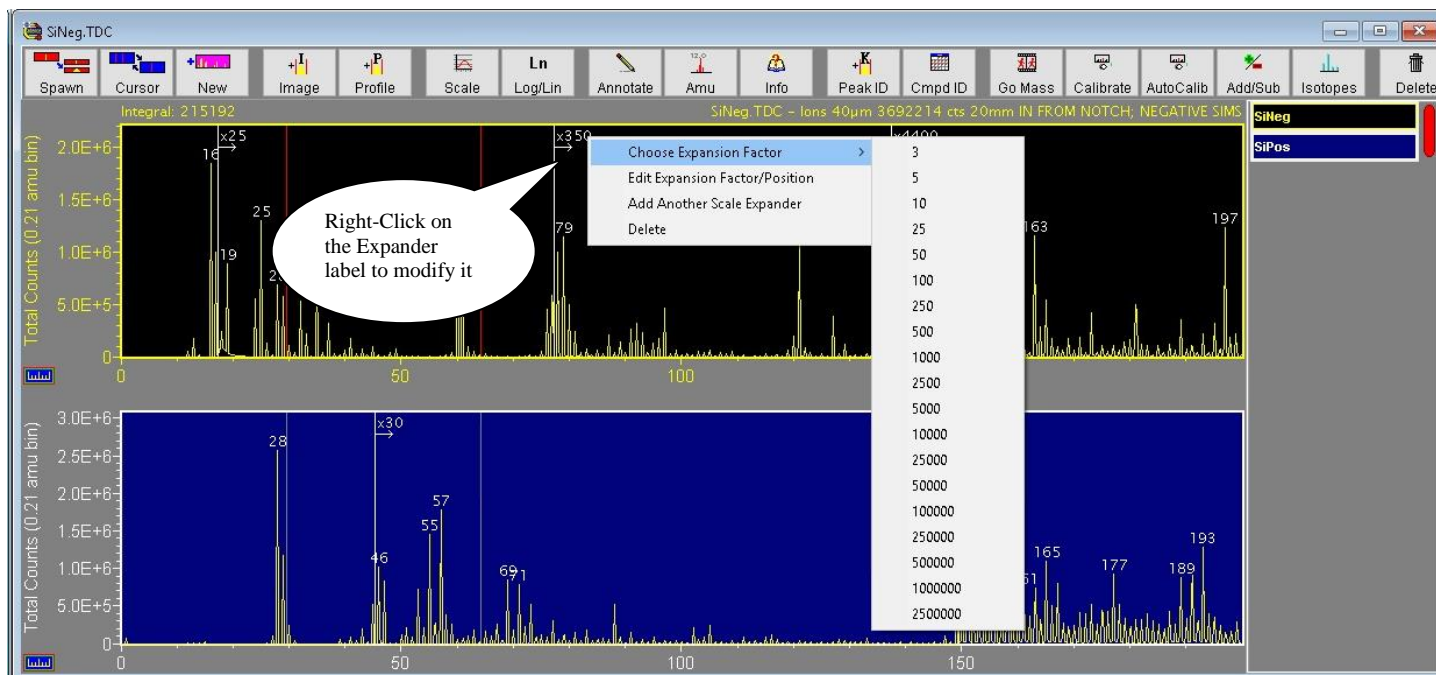


Figure 2 – Right click on the Expander label to modify it

This context menu includes the following items:

- Choose Expansion Factor provides a list of factors for quick selection.
- Edit Expansion Factor/Position allows editing of the Expander’s Factor and Position.
- Add Another Scale Expander will place an additional Expander on the graph
- Delete will remove this Expander from the graph.

To change the position of the Expander, simply drag (via the left mouse button) the label and drop it at the desired location, as shown below:

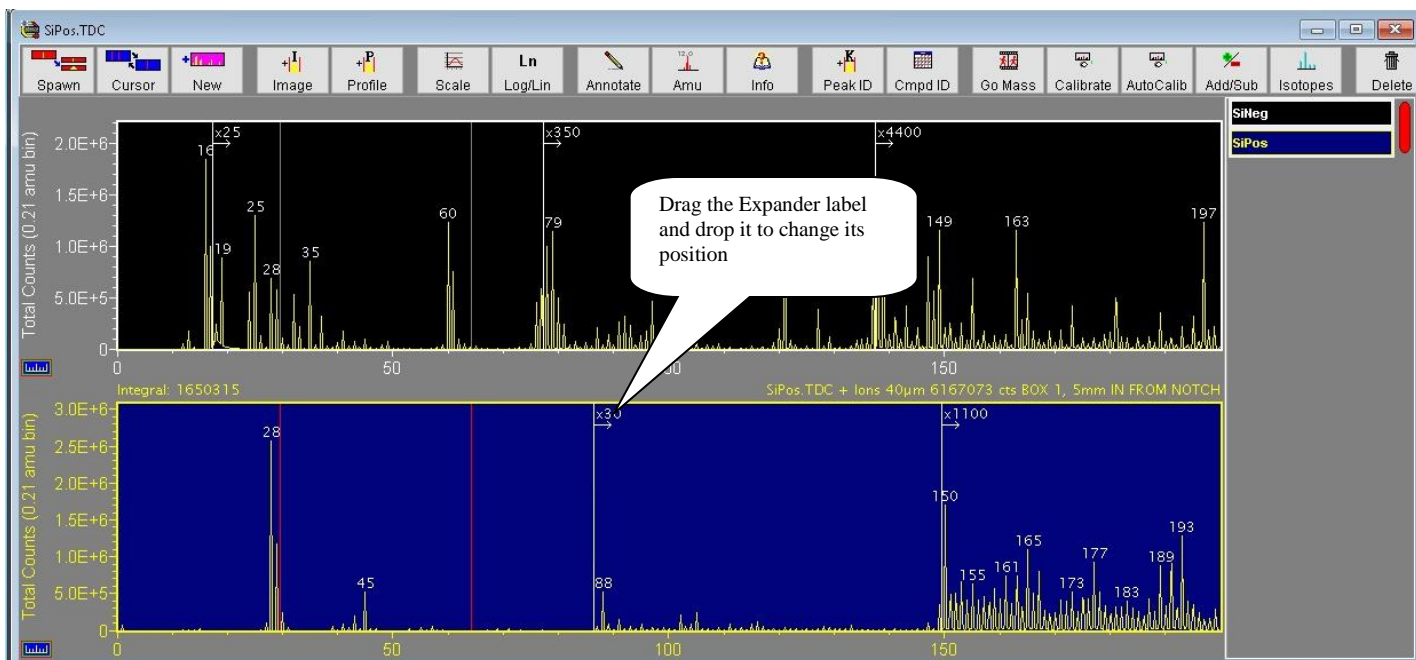


Figure 3 – Drag the Expander label to change its position

Note: To apply expanders manually, it is best (but not required) to uncheck the “Place Expanders Automatically” menu item on the Spectra | Intensity Scale Expanders sub-menu, which can be seen in the figure below.

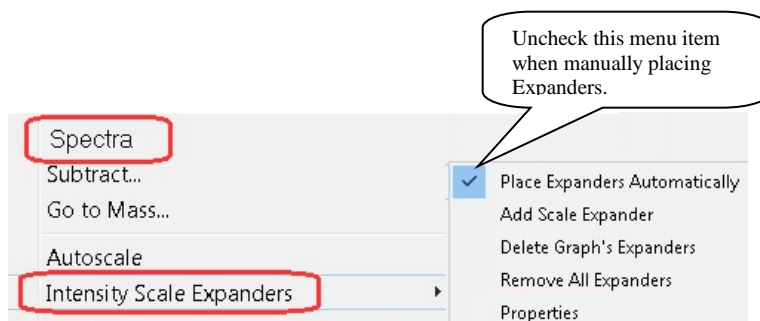


Figure 4 – The Intensity Scale Expanders sub-menu

Also on this submenu are the following items:

- The Add Scale Expander item will attempt to add a new Expander to the graph.
- The Delete Graph's Expanders item will remove any Expanders from the currently selected graph.
- The Remove All Expanders item will remove all Expanders from all graphs.
- The Properties item will be described below.

3. Applying Expanders Automatically

The normal AutoScale mechanism will apply expanders automatically with no extra effort from the user. This automatic placement feature can be turned on or off via the “Place Expanders Automatically” menu item on the Spectra | Intensity Scale Expanders sub-menu (see figure).

Also on this menu is the Properties item, which brings up a dialog as shown in the figure below.

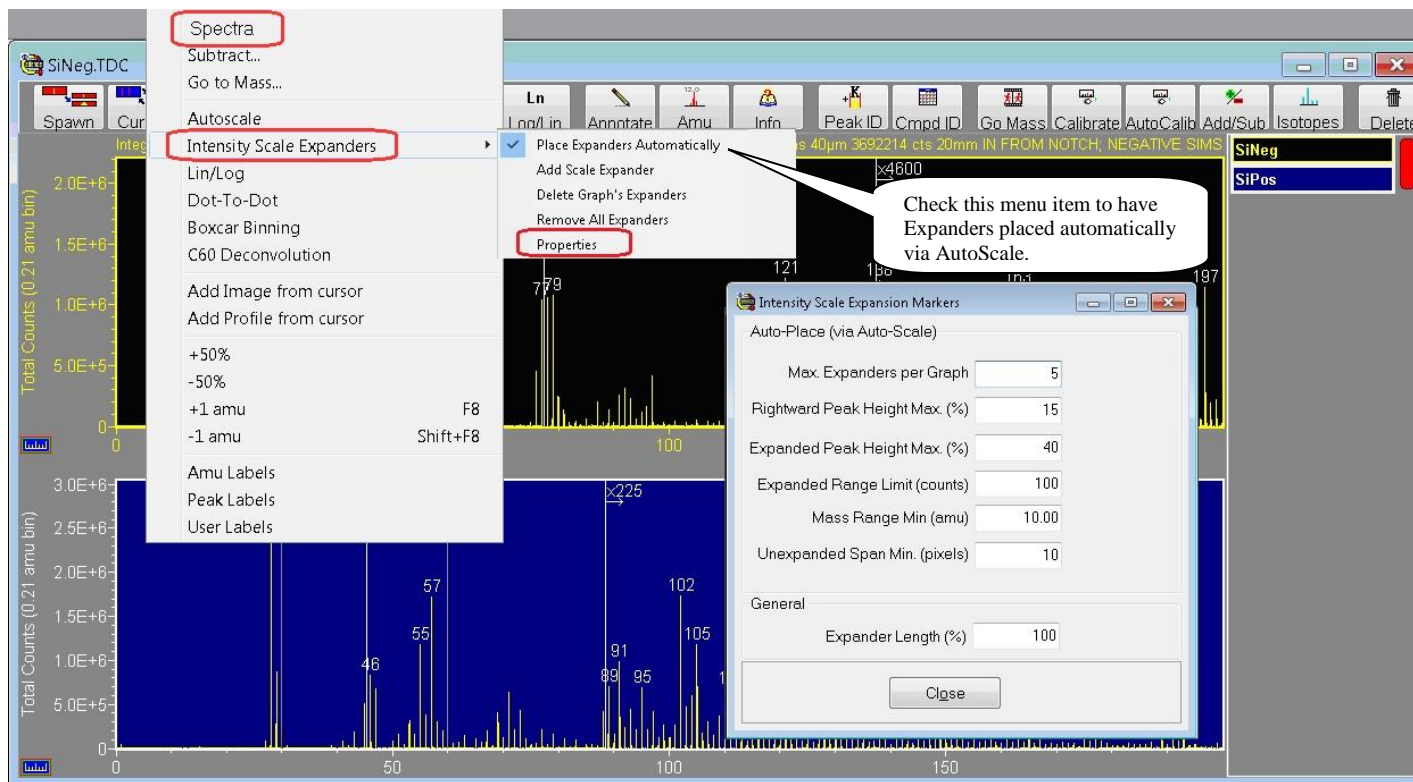


Figure 4 – Properties Dialog for Expanders

In the “Auto-Place (via Auto-Scale)” section is a set of properties that may be modified by the user in order to customize how expanders are automatically applied, and these are described below:

- The Max. Expanders per Graph value limits the number of Expanders that may be auto-placed on any graph. Note that although this is the absolute maximum limit, the properties below also impact (limit) the number auto-placed. It is recommended to begin with a value of at least 4 in order to get a feel for the effect of modifying the auto-place properties below. Note that auto-place may be turned off with a value of zero.
- The Rightward Peak Height Max (%) value determines how aggressively the AutoScale mechanism will try to place Expanders, and it is the most important of these properties. Larger values will cause more Expanders to be placed (and closer together). Lower values will cause fewer Expanders to be placed (and further apart). It is recommended that you experiment with this number as a starting point.
- The Expanded Peak Height Max (%) value will determine how tall will be the auto-scaled peaks rightward of the auto-placed Expander. Larger values will cause the Expander to have a larger factor value, so that peaks in the expanded range are taller.
- The Mass Range Min (amu) value sets the minimum amu range for auto-placing an Expander. Choosing a value of 10 for example, no Expander will be placed within a mass range less than 10 amu -- and this applies in terms of both the graph's entire mass range, and of proximity to another Expander.
- The Unexpanded Span Min (pixels) value determines the minimum separation between the left-most Expander and the graph's left side. Generally speaking, it is undesirable for an Expander to appear 'too close' to the graph's left side.
- The Expanded Range Limit (counts) value will prevent AutoScale from 'over-expanding' single-count peaks, because it is undesirable for single-count peaks to appear 'too tall'. Smaller values for this limit will allow single-count peaks to stretch taller.

4. General Properties

- The Expander Length (%) value will determine the Expander's vertical line length. This vertical line extends downward from the top of the graph to a distance determined by this percentage, where 100% indicates the entire graph height.

5. MSMS Expansion Markers

For MSMS spectral data, Expanders are also supported, and note that they operate in the leftward direction as shown in the figure below:

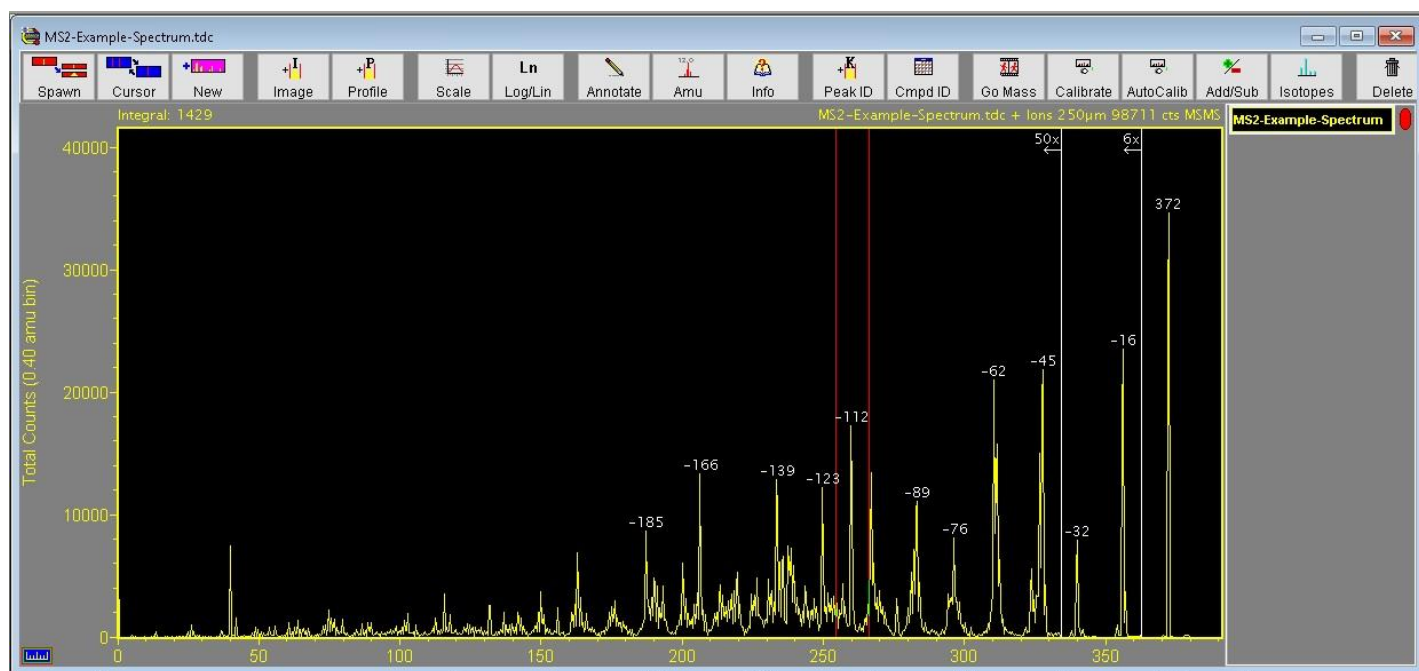


Figure 5 – Expanders operate in the leftward direction for MSMS data

VII. Peak-Groups in TOF-DR – Release Notes

TOF-DR Version 1.4

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1. Peak-Groups Overview

A peak-group enables the signal from several related ion species to be summed together into a single image, or profile-curve, or 3D-image.

This can be helpful to group isotopes together, or to boost signal-to-noise for any set of related ion species. For example, the three “child-peaks” of $^{28}\text{Si}^+$, $^{29}\text{Si}^+$ and $^{30}\text{Si}^+$ can be grouped together into a single “ $\Sigma^{28}\text{Si}^{29}\text{Si}^{30}\text{Si}$ ” peak-group in the Peak Window as shown below.

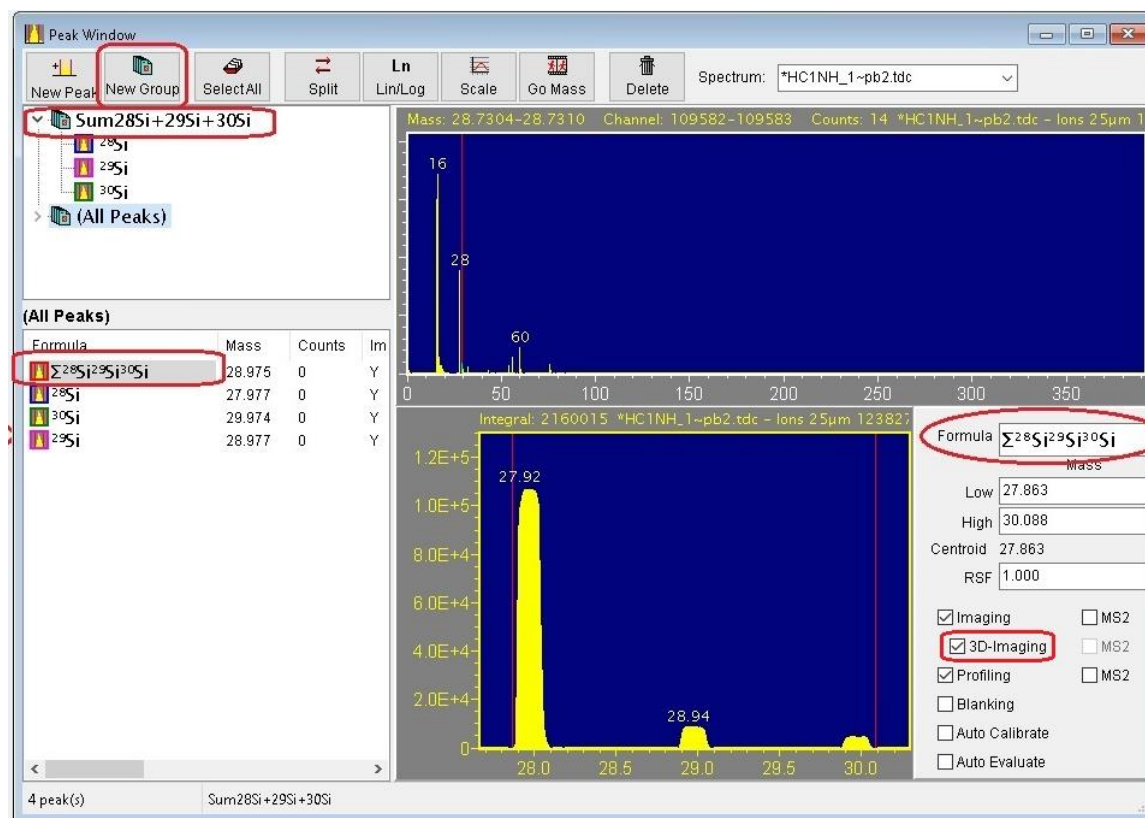


Figure 1 – Peak-Group defined in the Peak Window.

Note in the figure above that the '3D-Imaging' checkbox is checked for the peak-group.

When the next acquisition or raw data playback is complete, a 3D-Image for the group's summed signal will be created as shown in the figure below.

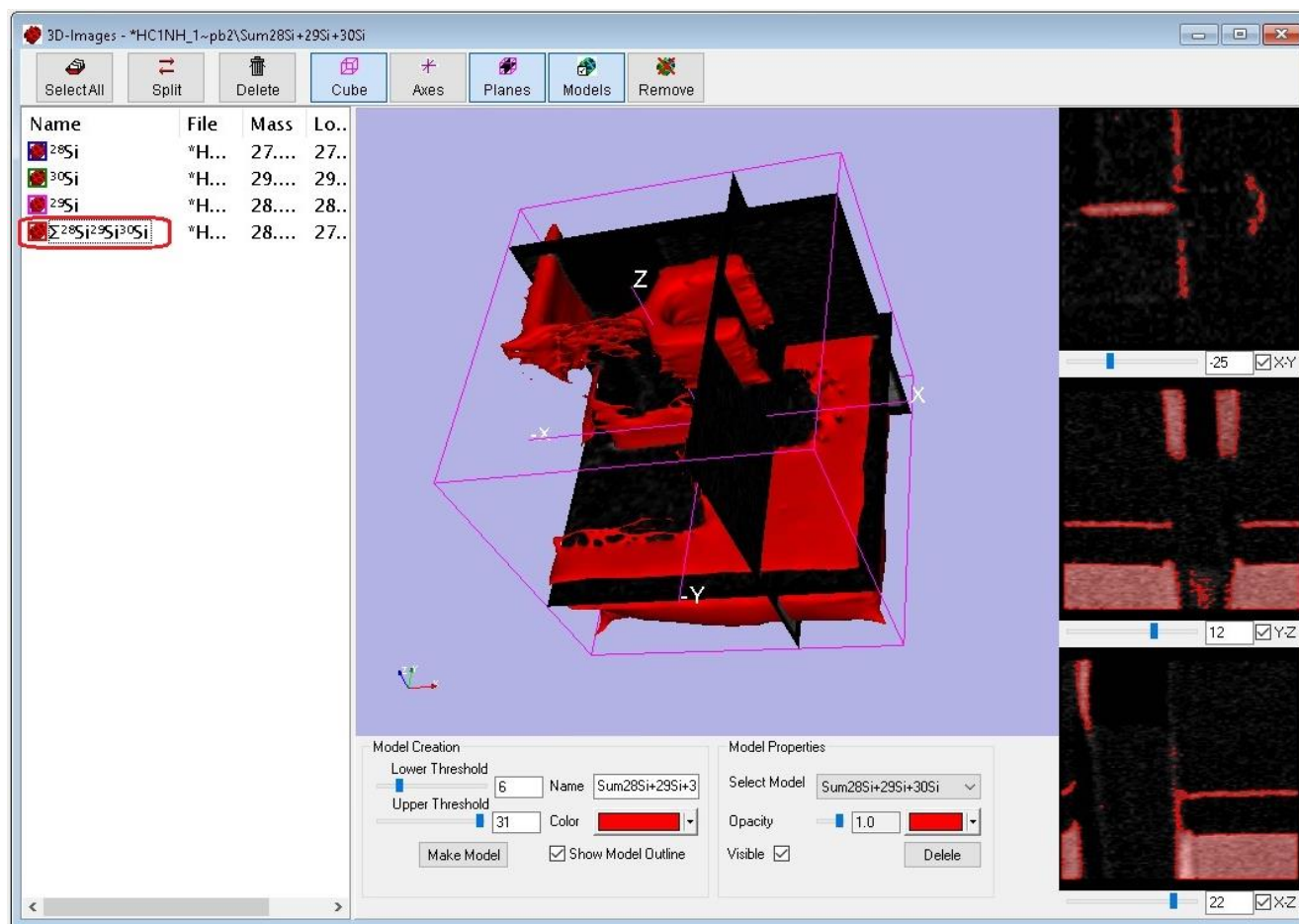


Figure 2 – 3D-Image of a Peak-Group

In the figure above, the ion signal from the three isotopes of silicon has been summed together into a single 3D-Image, and from this a solid model has been generated for display.

2. Defining a Peak-Group in the Peak Window

To begin defining a peak-group, in the Peak Window click the 'New Group' toolbar button, as shown in the figure below.

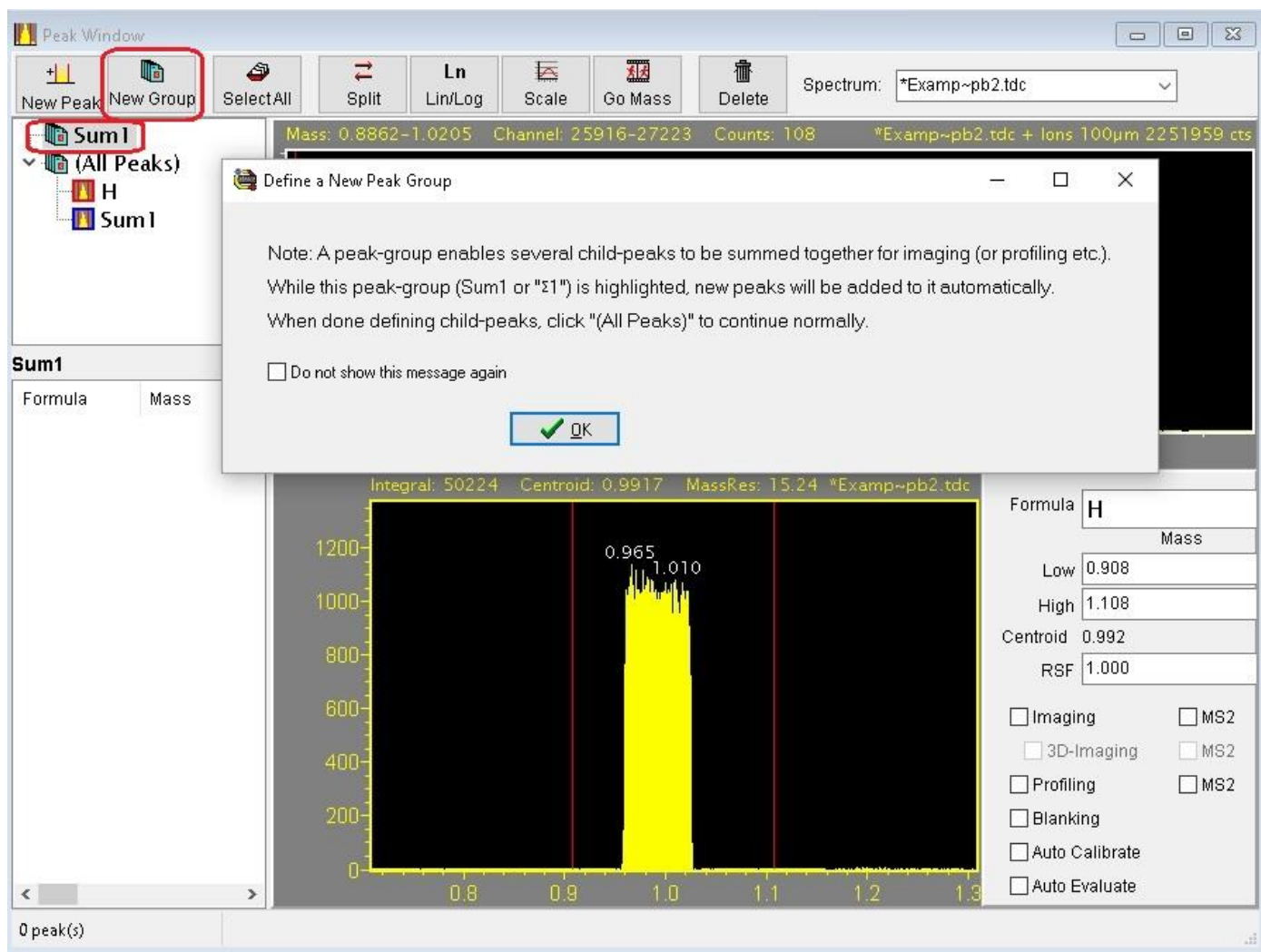


Figure 3 – Defining a New Peak Group

The new peak-group will be empty -- i.e. no child-peaks defined -- with an initial name like "Sum1" (or "Σ1") as shown in the figure. (An explanatory dialog box may appear with instructions as shown. Click the "OK" button on this dialog when you are ready to proceed.)

With the peak-group selected/highlighted in the tree-view (the upper view on the left-hand side) as shown, click the “New Peak” button and type a species name, e.g. “ ^{63}Cu ” as shown below

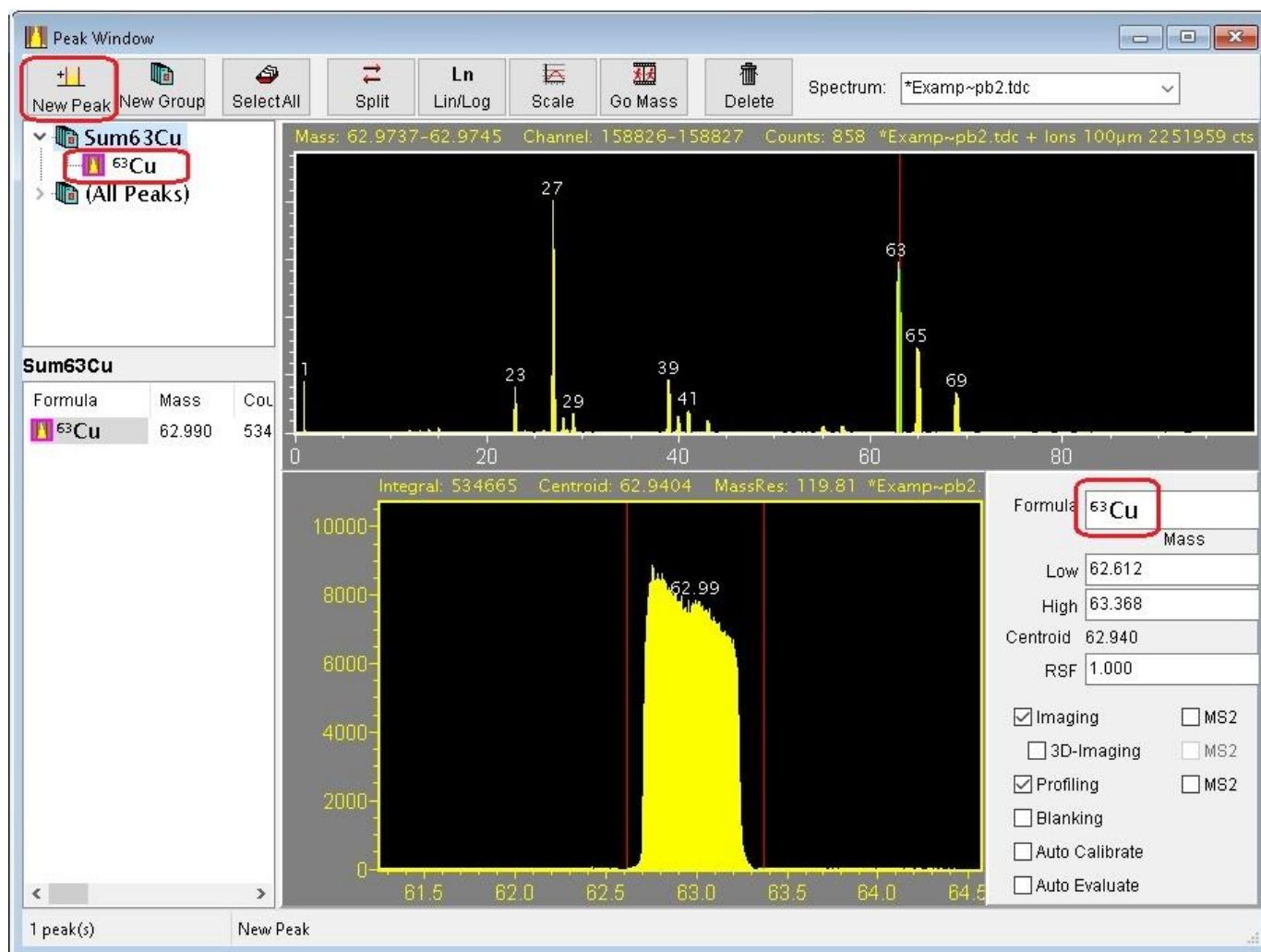


Figure 4 – Defining a 1st Child Peak for a Peak Group

The new child-peak is now the first child-peak defined for the peak-group. Note that the name of the peak-group will be updated automatically with a name like “Sum63Cu” (or “ $\Sigma^{63}\text{Cu}$ ”) as shown in the figure.

To define a second child-peak for this group, click the “New Peak” button again and type a species name, e.g. “ ^{65}Cu ” as shown below in Figure 5

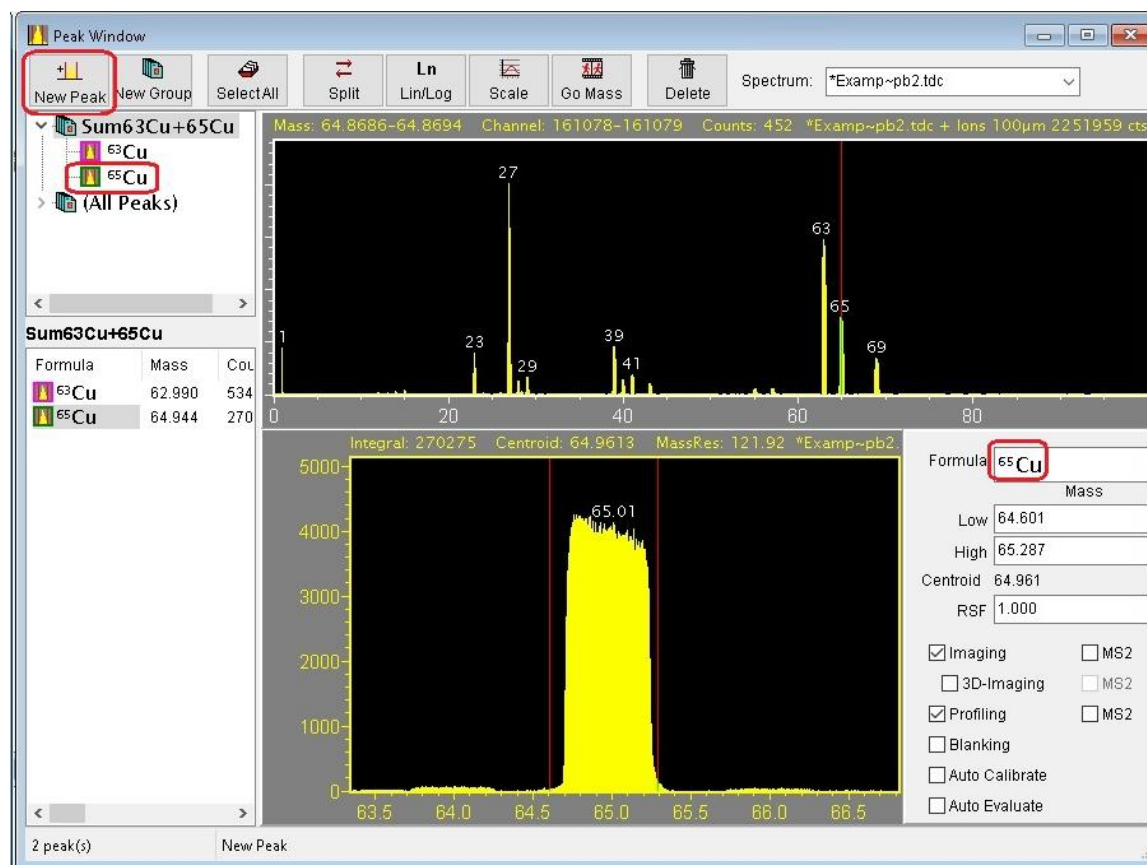


Figure 5 – Defining a 2nd Child Peak for a Peak Group

The peak group now has 2 child-peaks defined and the name of the peak-group will be updated automatically with a name like “Sum63Cu+65Cu” (or “ $\Sigma^{63}\text{Cu}^{65}\text{Cu}$ ”) as shown in the figure.

The user may modify the peak-group name as desired. It is recommended to use the “Sum” prefix -- for example “SumCu” or “SumGroup1” – but this is not a requirement.

3. Setting the 'Profiling' property for a Peak-Group in the Peak Window

Now that a peak-group with child-peaks is defined, click "(All Peaks)" in the tree-view (the upper view on the left-hand side), and this will cause all the peaks and peak-groups to be seen in the list-view (the lower view on the left-hand side) as shown below in Figure 6.

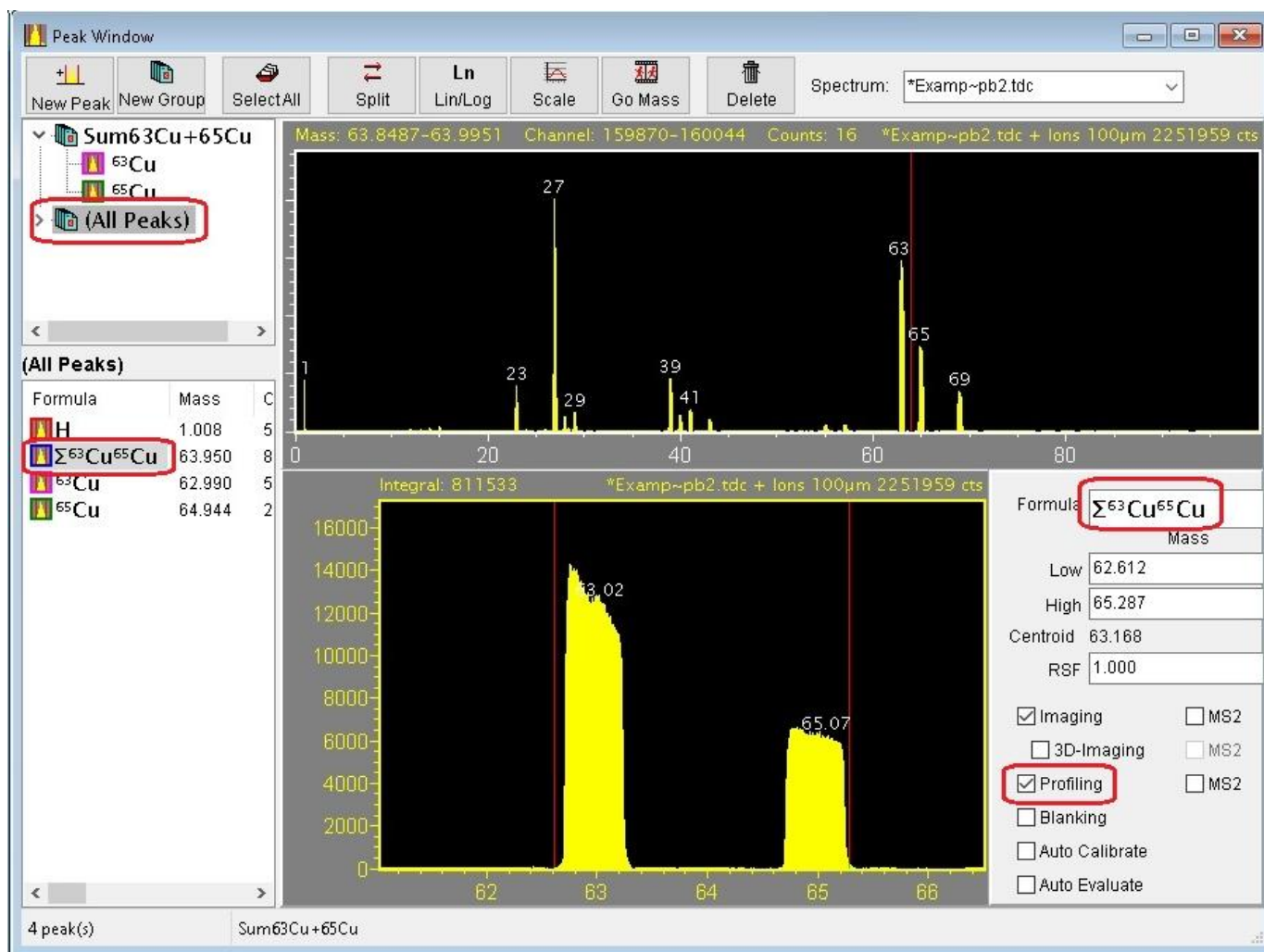


Figure 6 – Setting the Profiling property for a Peak Group

Now click the " $\Sigma^{63}\text{Cu}^{65}\text{Cu}$ " peak-group in the list-view, as shown in the figure above. On the right-hand side of the window you can select the checkboxes for Imaging/Profiling/3D-Imaging etc. for the peak-group in the same way as for any normal peak. Check the 'Profiling' checkbox in order to designate the peak-group for profiling.

Note that the red double cursor is shown in the figure above extending from the left side of the lowest mass child-peak to the right side of the highest mass child-peak, however the actual integration bounds that will be used for the peak-group includes only the set of child-peak sub-ranges (i.e. excludes everything outside these child-peak sub-ranges).

When the next acquisition or raw data playback is begun, a profile curve for the peak-group's summed signal will be created as shown in the figure below.

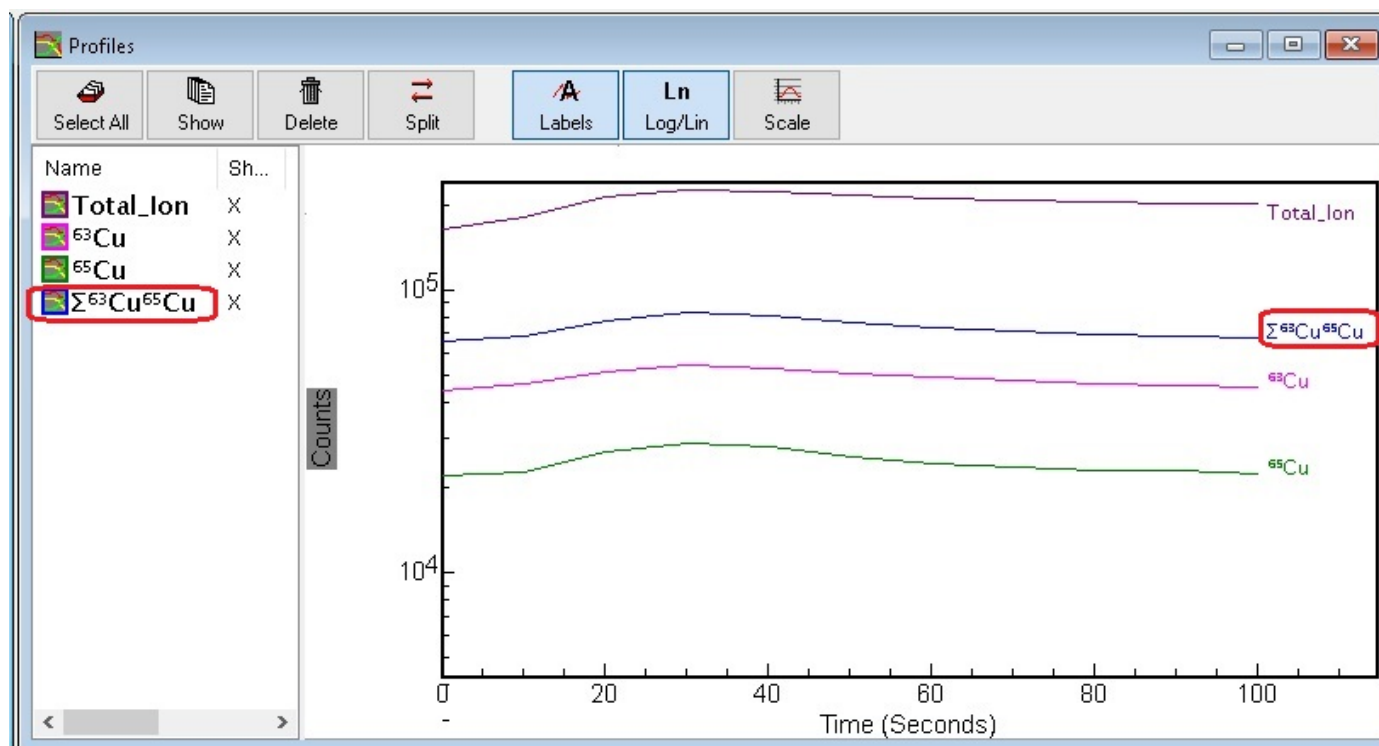


Figure 7 – The Peak Group Profile Curve shown in the Profiles Window

And the same procedure may be used to obtain Images / 3D-Images etc. for the peak group.