TOF-DR Software Release Notes

Contents

Release 4.0.0 – December 2024 (Win11; 64-Bit)

I. Introduction

In this release of TOF-DR, a new set of 3D visualization capability is available from the 3D-Image Window, including perspective view rendering with adjustable opacity and color scaling (described below in sections II thru IV).

Also, the ACE (Access Database Engine) driver is now always re-installed automatically at TOF-DR startup by default (described below in section V).

II. Perspective View Rendering

Below is an example of Perspective View Rendering for 3D depth profile data of Si, O, and H, and the fourth rendering is an overlay of all three.

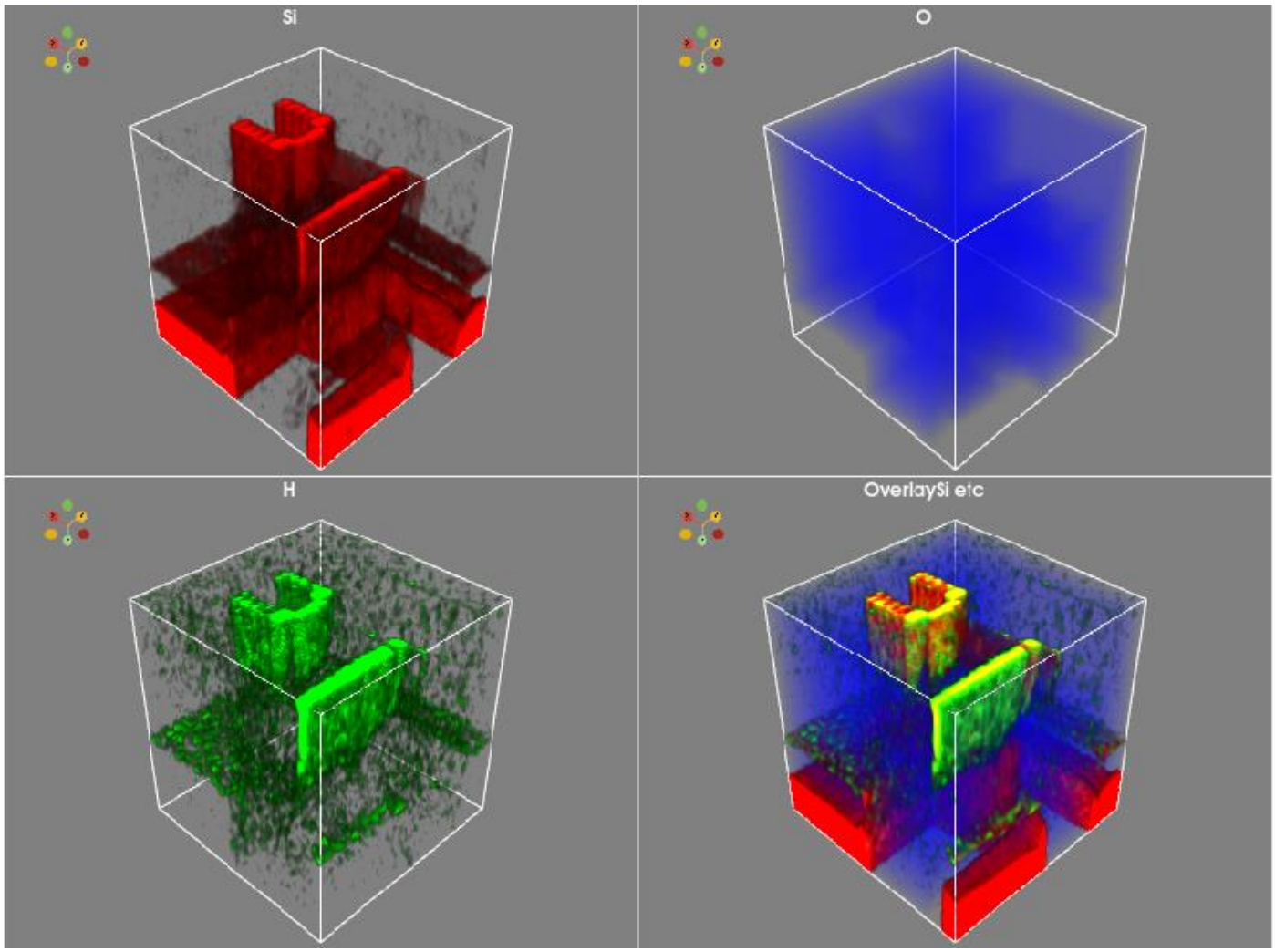


Figure 1 –.Perspective View Renderings of Si, O, H and Overlaid

Below is a more detailed Perspective View Rendering of the overlaid image from a different viewing angle, which shows scaled axes and demonstrates the application of opacity in its ray tracing.

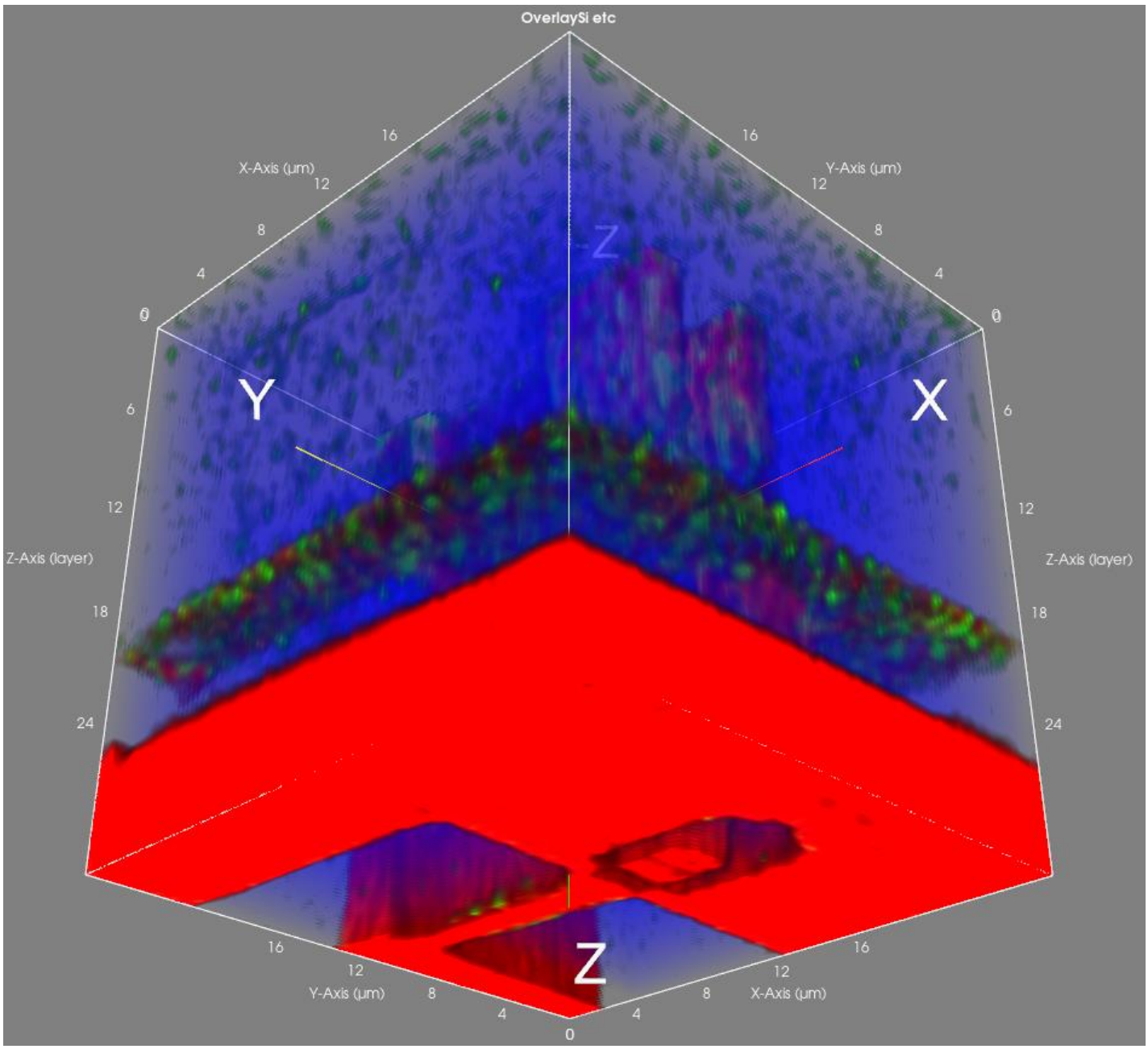


Figure 2 – Perspective View with Axes

III. The 3D-Images Window

On the TOF-DR main menu, choose the **Window|3D-Images** option to bring up the 3D-Images window. To follow along with the discussion below, choose the **File|Open-3D-Images menu** option from the TOF-DR main menu, navigate to the **Examples** folder in the TOFDR installation folder (typically this will be **C:\TOF-DR\Examples**), choose the **3D-Images.3DI** file and click **Open** to display the data.

The 3D-Images Window is shown below:

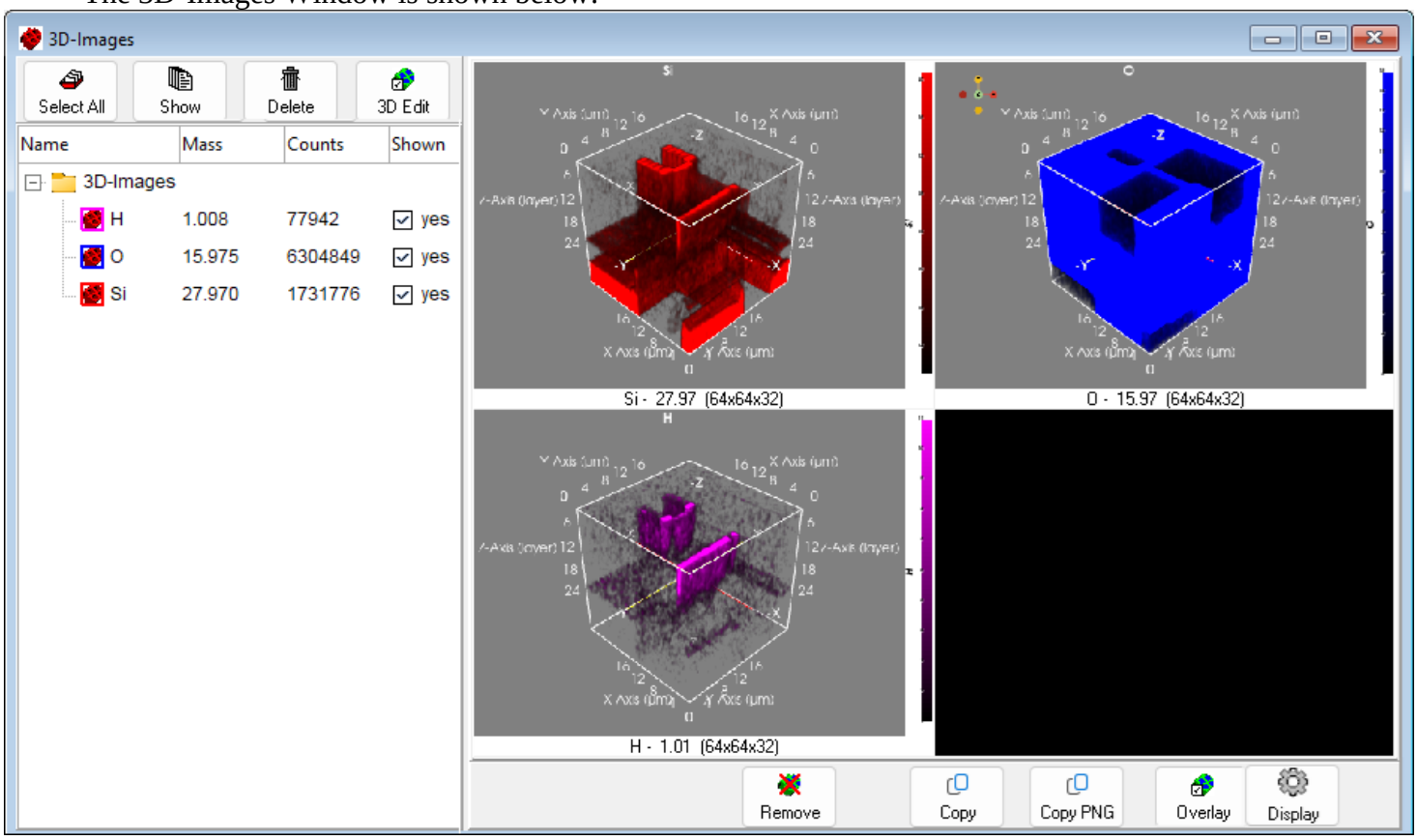


Figure 3 – 3D-Images Window (simplified for clarity)

The 3D-Images window displays a tree-view on the left side, and a grid of tiles (each displaying a perspective view image) on the right side. (Note that the image in Figure 3 is simplified to show a grid of 4 tiles for clarity, whereas the window normally displays 12 tiles in a 3x4 grid.)

Click on a species in the tree-view, or on a tile in the grid, to select it. Use Ctrl key and mouse-click to multi-select.

Beneath the grid tiles is a toolbar with the following buttons:

Remove – Empty the current tile of its perspective view image.
Copy – Copy the perspective view image to clipboard.
Copy PNG – Save Copy of perspective view to a .PNG image file.
Overlay – From the multi-selected grid tiles, create a new overlaid perspective view
Display – Open the 3D Display Options Dialog. Shown below

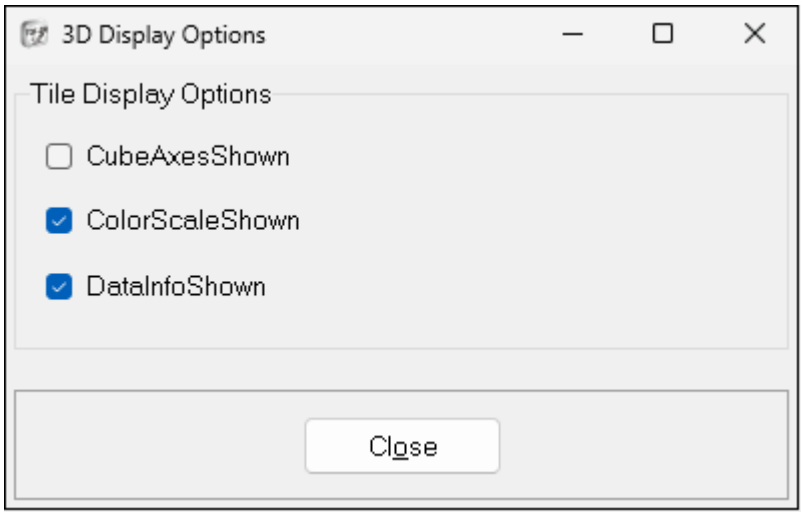


Figure 4 –3D Display Options Dialog

Set the checkboxes in the 3D Display Options Dialog as desired, and click Close to apply.

Right Click on any tile to bring up a context menu with the following options:

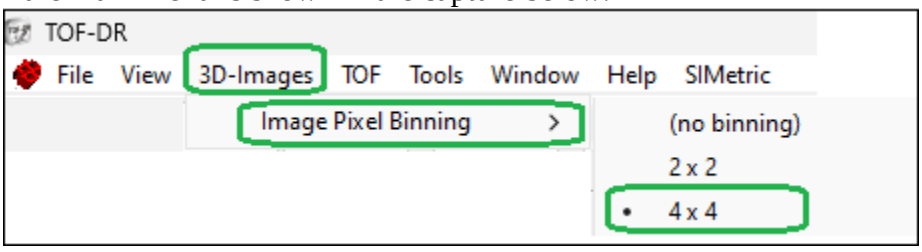
Edit in 3D – Launch the 3D Editor dialog for the grid tile.
Copy to Clipboard – Copy the grid tile to the clipboard.
Save as 3D-Images (.3DI) File – Save the grid tile to a .3DI file.

Above the tree-view is a toolbar with the following buttons:

Select All – Select all items in the tree view
Show – Show the selected item in the tree view in an empty grid tile
Delete –.Delete the selected item from the tree view
3D-Edit – Launch the 3D Editor dialog for the selected item in the tree view

Note that 3D-Species items may be dragged from the tree view onto an empty grid tile in order to display the perspective view.

XY Image Pixel Binning – It is sometime desirable to increase signal to noise in the 3D-Images by merging (summing together) multiple pixels into a single pixel. In the main menu, when the 3D-Images Window has focus, choose **3D-Images|Image Pixel Binning** in order to select how XY pixels are binned when 3D-Images are loaded (or created via raw playback) in the future. This menu option in the main menu is shown in the capture below.



In the capture above, '**4 x 4**' is selected, which indicates that TOFDR will merge 16 pixels into a single pixel when 3D-Images are loaded in the future. In this way, if the original image was acquired with a resolution of 256x256 pixels, then with 4x4 binning, then the 3D-images will have 64x64 pixels in XY, and the pixels will have greater intensity and the image will exhibit better signal to noise. Note that changing this value will affect 3D-Images loaded (or created via raw playback) in the future (current 3D-Images in the tree-view and tile grid will not be affected).

IV. 3D-Image Editor Dialog

In order to adjust the viewing angle and the data appearance of the 3D perspective view, use the 3D-Image Editor dialog, which is shown below.

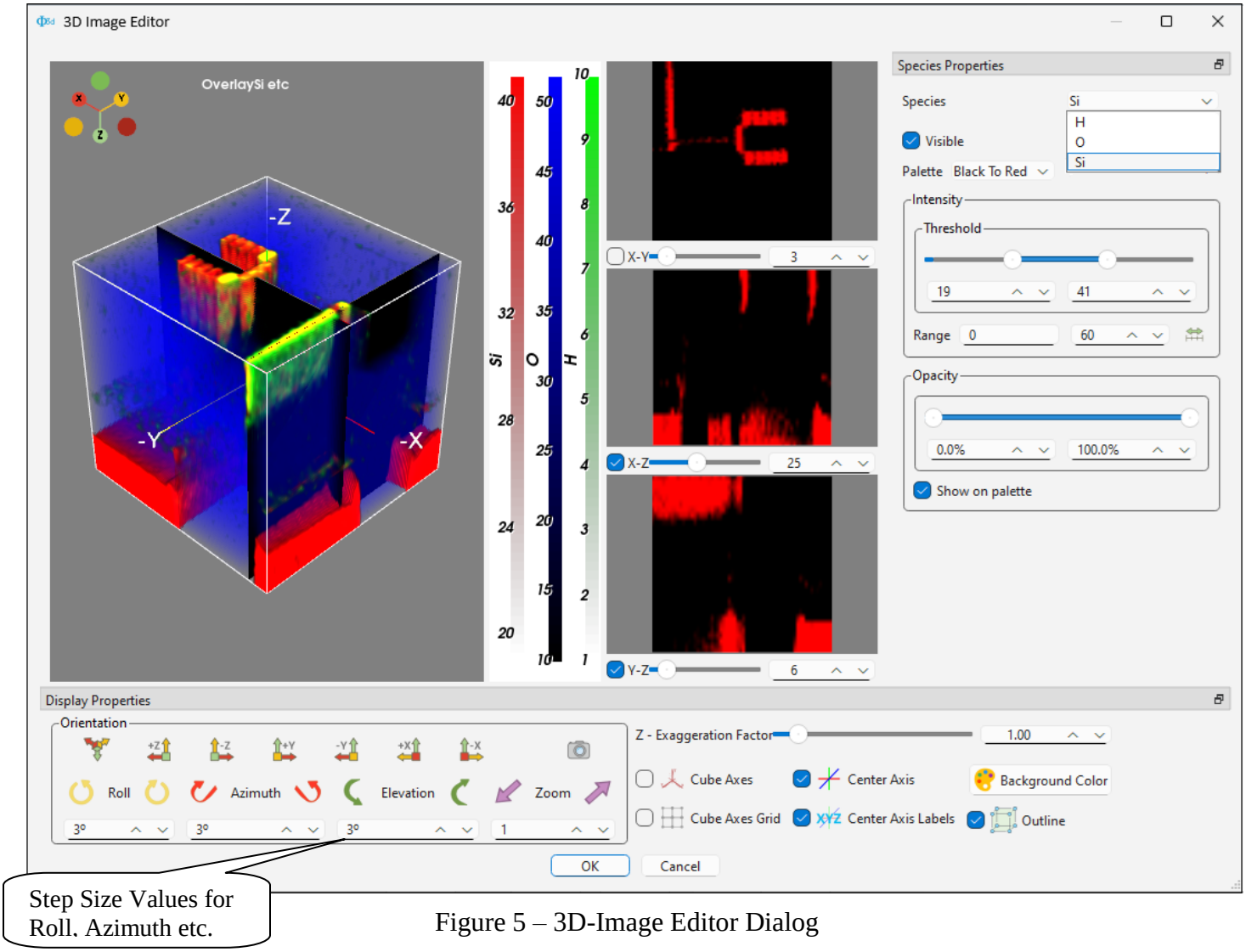


Figure 5 – 3D-Image Editor Dialog

On the left side of the dialog is the 3D View – change the viewing angle orientation in real time via mouse click and drag:

- Left Drag – tilt and rotate
- Left Drag with Ctrl key – roll clockwise/counter-clockwise
- Left Drag with Shift key – translate (shift) up/down left/right
- Left Drag with Ctrl Shift key – zoom in out

To the right of the 3D-View is the area for color scale(s) – In Figure 5 Si is shown with a red color palette and an intensity scale range from 19 to 41, O with blue and a scale range from 10 to 50, and H with green and a scale range from 1 to 10 – note that other colors (orange, yellow) appear in areas where Si and H overlap.

On the right side, are the Species properties – when multiple species are overlaid, choose a particular species from the Species drop-down (Si is shown selected in Figure 5) in order to set the Intensity Threshold, Opacity etc for that species.

Visible checkbox – when unchecked, this species will be entirely transparent/unseen.

Palette dropdown – choose a color palette such as 'Black to Red' or 'Cold and Hot' etc.

Intensity group

Within the **Intensity** group is the following:

Threshold -- Low and High, use the slider or spin box to adjust the color scale range. In Figure 5, the threshold for Si is shown with Low=19 and High=41. These values define the range of the color scale (seen in the color scale area) for Si, and indicate which color in the palette corresponds to a particular intensity (e.g. in Figure 5, pixels with intensity of 41 or higher are rendered with the most intense color of red).

Range -- Low and High – Expand the range of the Threshold slider/spin-box by adjusting the High value to a larger number.

Range Reset Button  -- resets the range to the default values

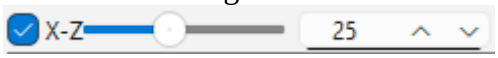
Opacity group

Within the **Opacity** group is the following:

Opacity -- Low and High, use the slider or spin box to adjust the opacity range, which determines how transparent a pixel is when 3D ray tracing is applied. In Figure 5, the opacity for Si is shown with Low=0 and High=100. These values are applied linearly to the intensity threshold range shown in the color scale (e.g. in Figure 5, pixels with intensity of 41 or higher are rendered opaque, while pixels with intensity of 19 or lower are rendered entirely transparent).

Show on palette checkbox – when checked, opacity is incorporated into the color palette when it is rendered on the color scale in the color scale area.

The middle of the dialog shows the 3 slice-plane views with XY at the top, XZ below that and YZ beneath. Beneath each of these are the following:



Slice-Plane spin box – sets the pixel number of the slice plane.

Slice Plane slider -- sets the pixel number of the slice plane.

Slice-Plane checkbox – When checked, the selected slice plane number will be shown rendered on the 3D-View (at left) as a black planer surface. For example in Figure 5, the XZ value is 25 and YZ value is 6 and both of these are rendered as a black planer surface in the 3D-View.

The bottom of the dialog shows the Display properties, with Orientation controls and checkboxes as described below.

Within the **Orientation** group is the following:

A series of preset orientation buttons are provided

These buttons instantly snap the 3D-View to a particular orientation

A series of preset orientation-step buttons, and their corresponding step size spin boxes.

These orientation step buttons will step the orientation of the 3D-View in a particular manner. For example the Elevation step buttons will tilt the 3DView up and down. The step size for these buttons is adjustable via the spin box. For example the step size for the Elevation step buttons can be changed from the default (3 degrees) to a larger value such as 20 degrees.

Z-Exaggeration Factor spin box and slider – Adjust the Z-scaling thicker/thinner in the 3D-View
Cube Axes Checkbox – Show Cube Axes in the 3D-View
Cube Axes Grid Checkbox – Show Cube Axes Grid in the 3D-View
Center Axis Checkbox – Show Cube Axis for XYZ in the 3D-View
Center Axis Labels Checkbox – Show Cube Axis Labels ('X, 'Y', 'Z') in the 3D-View
Background Color button – Choose a new background color;
Cube Outline Checkbox – Show the Cubic Outline in the 3D-View

To exit the dialog click the Ok or Cancel buttons at the very bottom of the dialog.

V. ACE (Access Database) Driver Installation

The ACE (Access Database Engine) driver is now always installed automatically at TOF-DR startup by default. This driver allows TOF-DR to search databases such as the Fragment Library, and CompoundID database. Reinstalling the driver at startup ensures that the correct version of the ACE driver is available and working properly for TOF-DR.

At TOF-DR startup, you will be explicitly requested to authorize the reinstallation of the ACE driver, and in this case you should answer **Yes/Reinstall/Ok** to ensure that the driver is reinstalled.

If for any reason, you do not wish to reinstall the ACE driver always at TOF-DR startup, this behavior can be turned off in the following way. Use Windows Explorer to navigate to folder location **C:\TOF-DR\Setting\GeneralSetup\Properties**, and right click on the text file **Properties.phi** , select the **Open with…** option, and from the list choose the Windows **Notepad** app. When the text for this file is displayed in the Notepad app, look for the line that says

InstallAceDbDriverAtStartup=True

And in that line, change the =True to be **=False** and save the file.

Release 3.4.0 – September 2023 (Win11; 64-Bit)

I. Introduction

In this release of TOF-DR, a number of new features have been added -- including the new 'Score ML' button, which applies Artificial Intelligence to provide a mass calibration confidence score – as well as a number of issues that have been corrected since the last release.

II. New Features & Corrected Issues

i) Mass Calibration Confidence Score via Artificial Intelligence

On the Mass Calibration form, the 'Score ML' button has been added. TOF_DR now provides this simple mechanism for go / no-go feedback of spectral calibration confidence via an algorithm using Artificial Intelligence empowered Machine Learning (ML). The algorithm involves a supervised approach for both feature identification (i.e., organic, atomic and isotope peaks) and classification (i.e., high or low confidence). This algorithm provides an ML Score of zero to 99% to classify the spectral calibration as "high confidence" or "low confidence". High confidence is defined as > 90% and low confidence is < 80%.

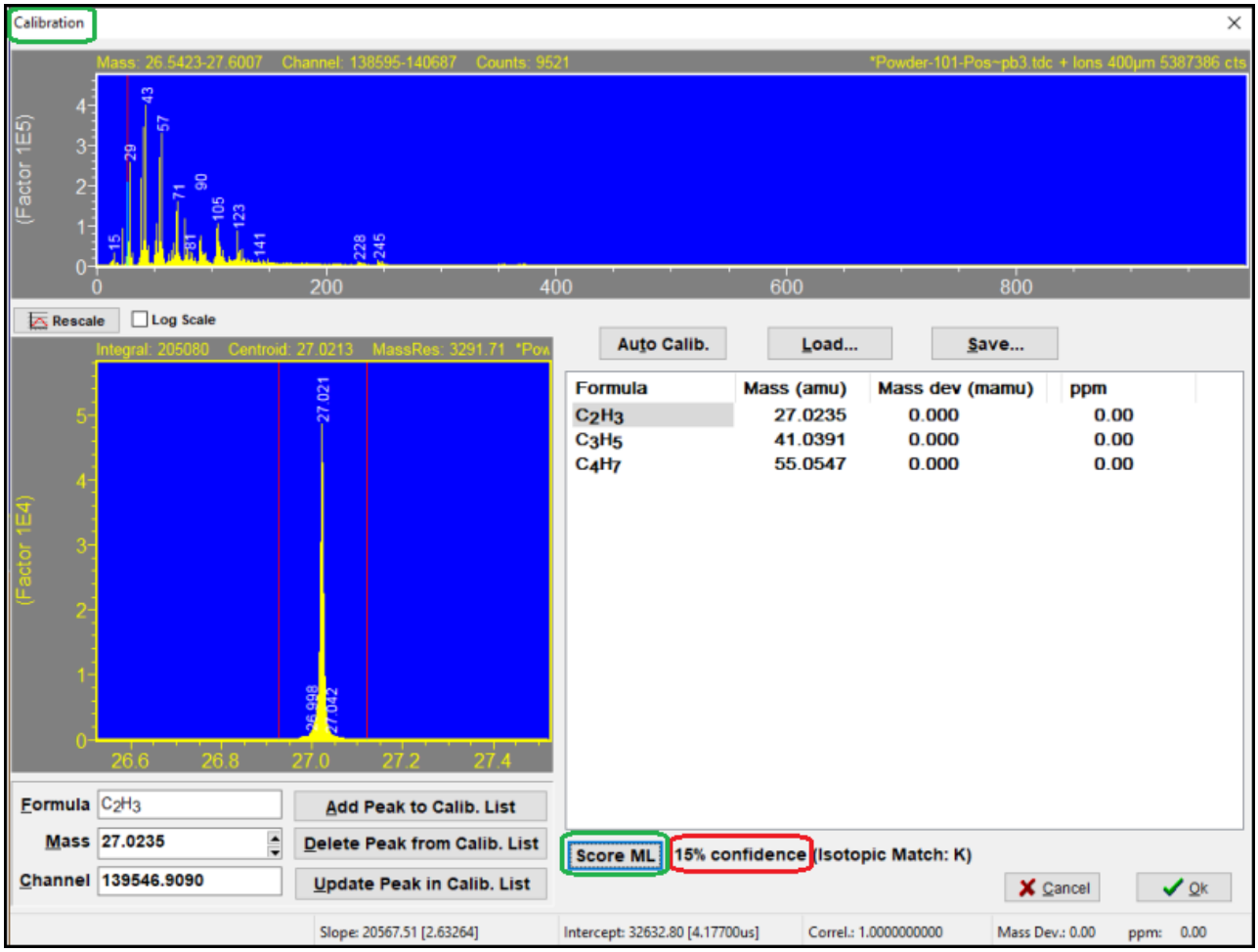


Figure 1 –The 'Score ML' button on the Mass Calibration form. The 15% ML Score indicates low confidence due to an uncalibrated spectrum or incorrect peak assignment(s).

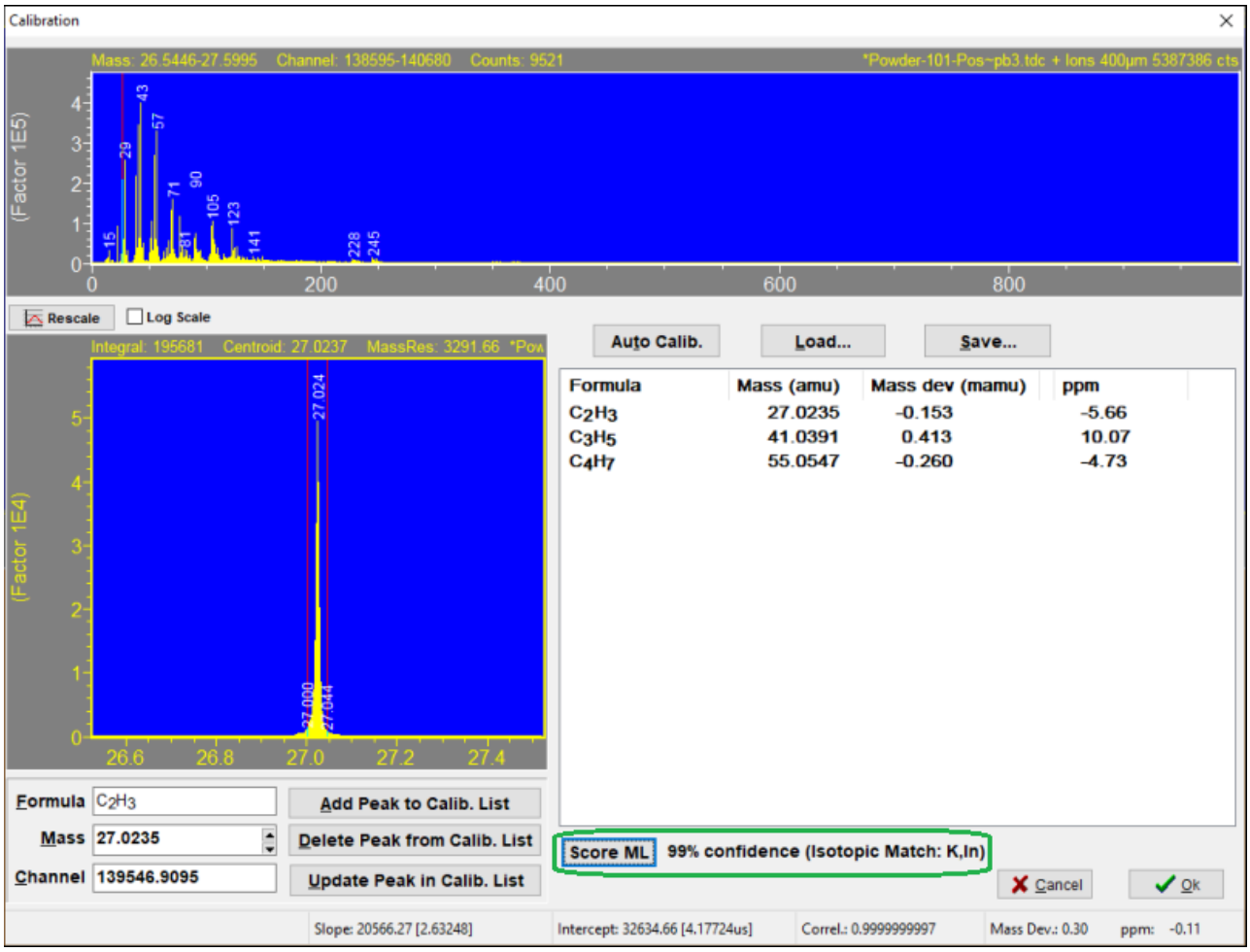


Figure 2 – The 99% ML Score indicates high confidence in the calibration and further indicates correct isotope ratios.

The example data shown in the Figures above illustrate the feedback provided by the ML Score, an indication of the confidence level of correct peak assignments in the mass calibration. In addition, TOF-DR will note any elements that approximately match the isotopic pattern of naturally occurring abundance (for example, in the figure above, we see “Isotopic Match: K, In) for this spectrum using this calibration.

ii) Intensity Scale Expanders Linked

Now when graphs are Mass-Linked in the Spectrum Window, the intensity scale expansion markers (expanders) are sync'd, which means that any expander modification on one graph will reflect likewise on the other graphs (e.g. addition/deletion/reposition-drag/factor-change etc.).

To test this feature in the Spectrum Window, first click the Mass-Link button in the normal manner in order to Mass-Link the axes, then click the 'Add Expander' toolbar button. Note that the new expander has been added to all mass-linked graphs. Now drag the expander label or change its factor or delete it, and note that the change is applied to all graphs.

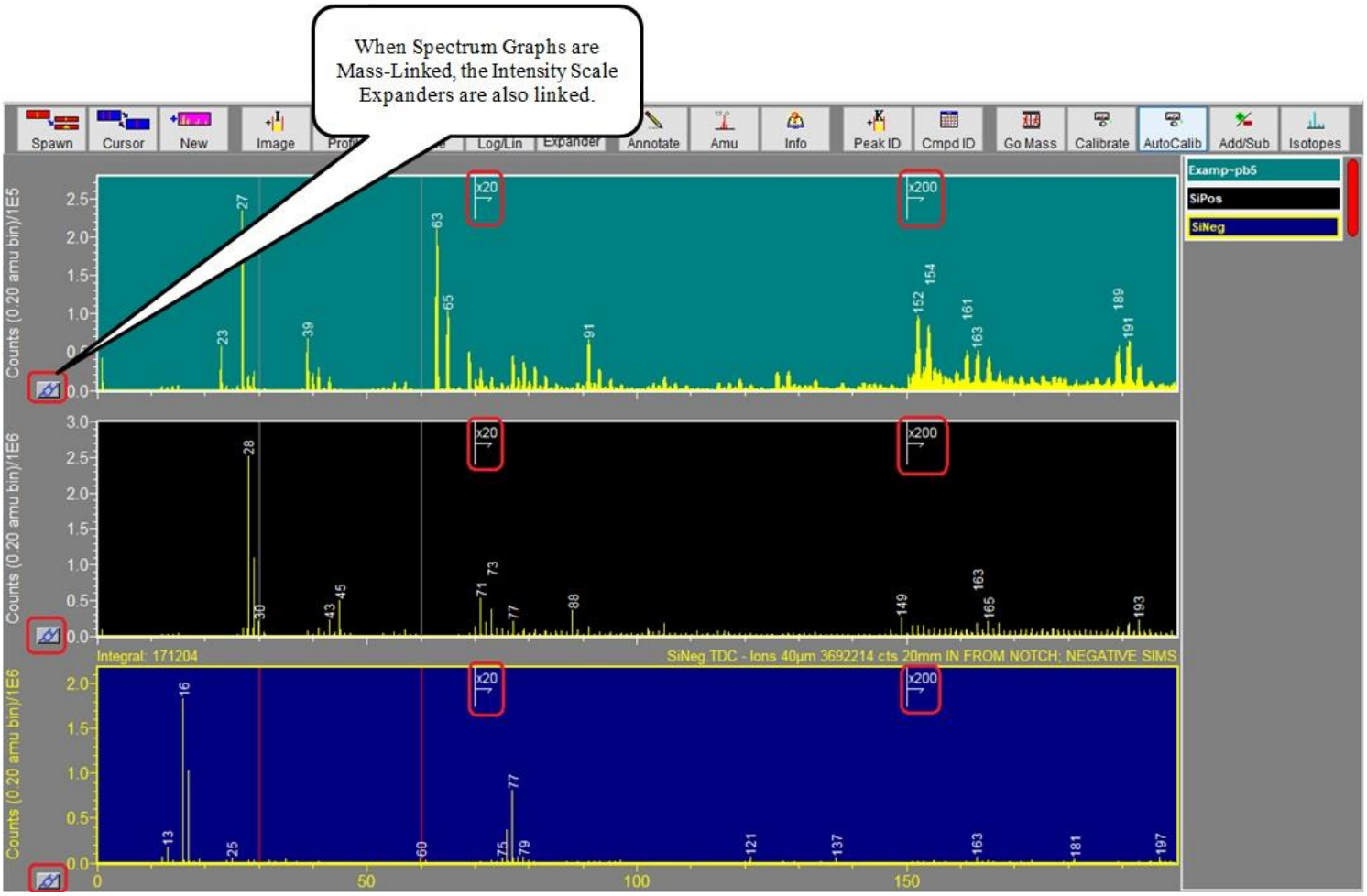


Figure 3 – Expanders are Sync'd when Graphs are Mass-Linked in the Spectrum Window

Notes:

When the user invokes Mass-Link (by clicking on the bottom graph's Mass-Link button), TOFDR will by default apply the bottom graph's expanders to the other graphs as a starting point; However if AutoPlace is on (i.e. if "Place Expanders Automatically" is checked in the Spectrum|Intensity Scale Expanders menu) and if the bottom graph is currently AutoScaled (i.e. the left axis AutoScale mode checkbox is checked), then TOFDR will attempt to AutoPlace Expanders in a way that is appropriate for all the graphs (using the normal AutoPlace rules) as a starting point.

Note that while graphs are Mass-Linked, clicking the AutoScale button on the toolbar will not cause expanders to be re-AutoPlaced (i.e. all expanders will remain unchanged) -- but when Mass-Link is turned off again, this AutoPlace capability will be restored as normal.

iii) Edit Compound Info in the CompoundID Database

The user may now edit or modify compounds that have been previously added to the default CompoundID database.

The user (after launching the CompoundID Window), on the 'Delete' tab, can right click on the compound of interest and choose 'Modify Compound in Database'. See the figure below:

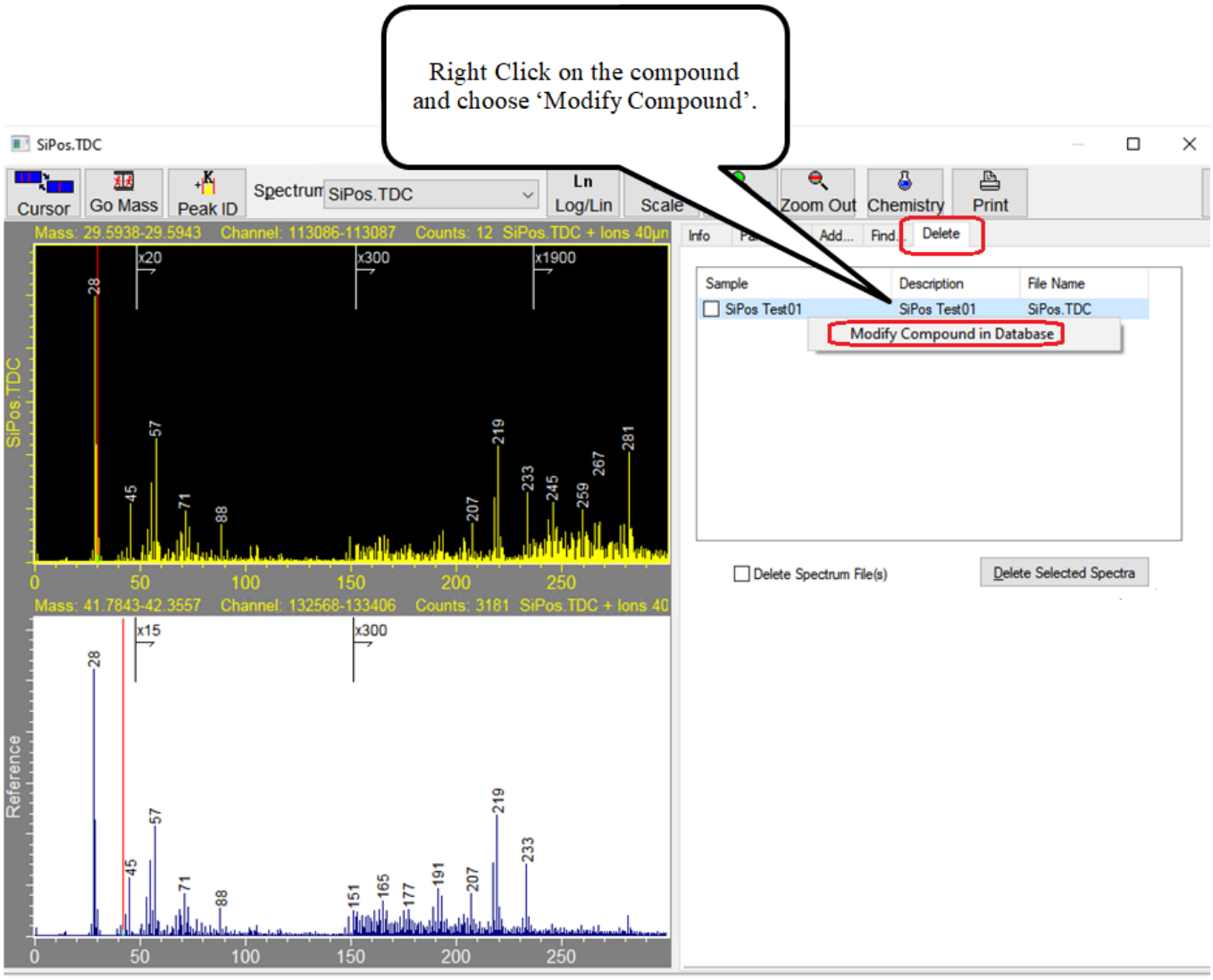


Figure 4 – Right Click on the compound and choose 'Modify Compound'.

A modal dialog will appear in which the user may make modifications and click Ok to save in the database. See the figure below:

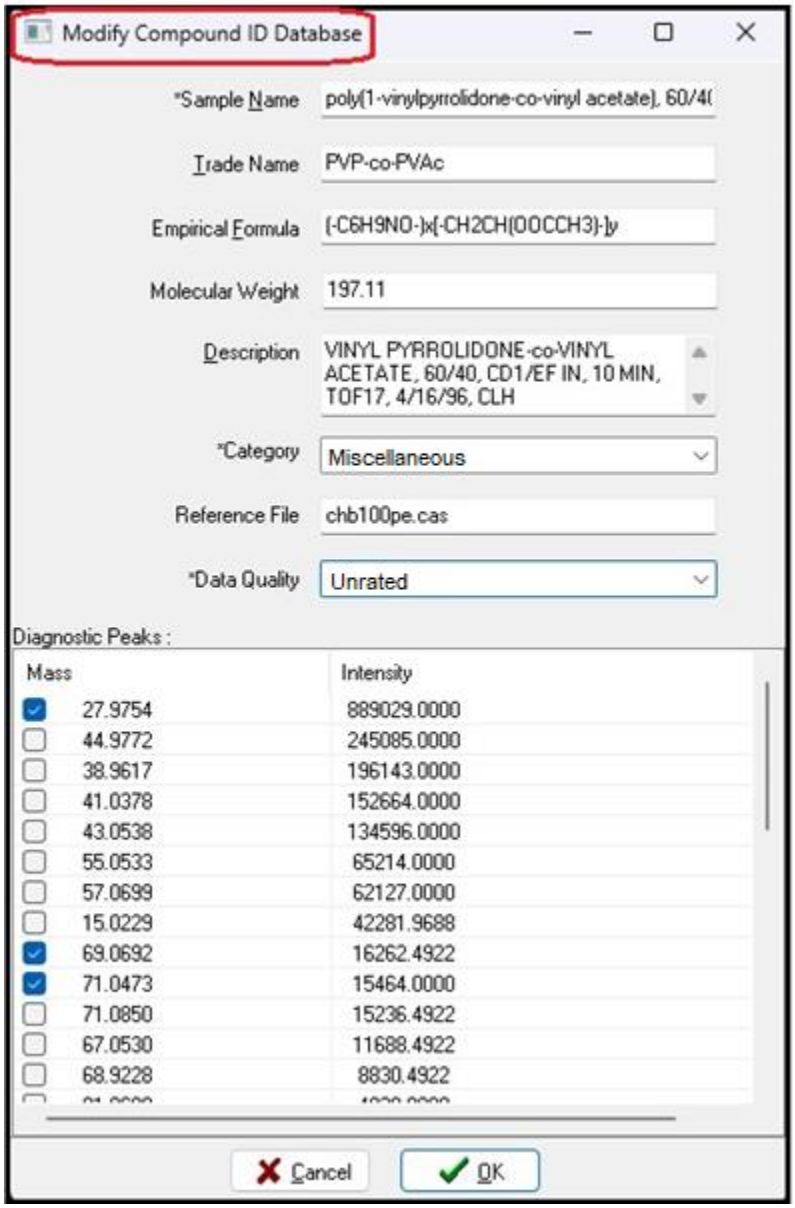


Figure 5 – Edit Compound Info in the CompoundID database

Note: for the 'Category' field, it is recommended to choose one of the already existing predefined categories (e.g. 'Electronic Materials' or 'Miscellaneous') from the dropdown; However, it is also possible to define an entirely new category name (i.e. so that it will be available as a choice in the dropdown in the future). To define an entirely new category name, type the new name into the Category combo-box, click Ok, and at the prompt "Do you want to add X as a new category in the database?", click Ok. A prompt will appear confirming that the new category has been added to the database. Note that TOFDR must be restarted for this change to be fully reflected in the Compound ID feature.

iv) Normalized Spectrum Display

In the Spectrum Window, a normalization method for Spectra may be chosen by the user.
From the Spectrum Window, choose the Spectra|Normalization menu option in order to display the Spectrum Normalization Dialog. See the figure below:

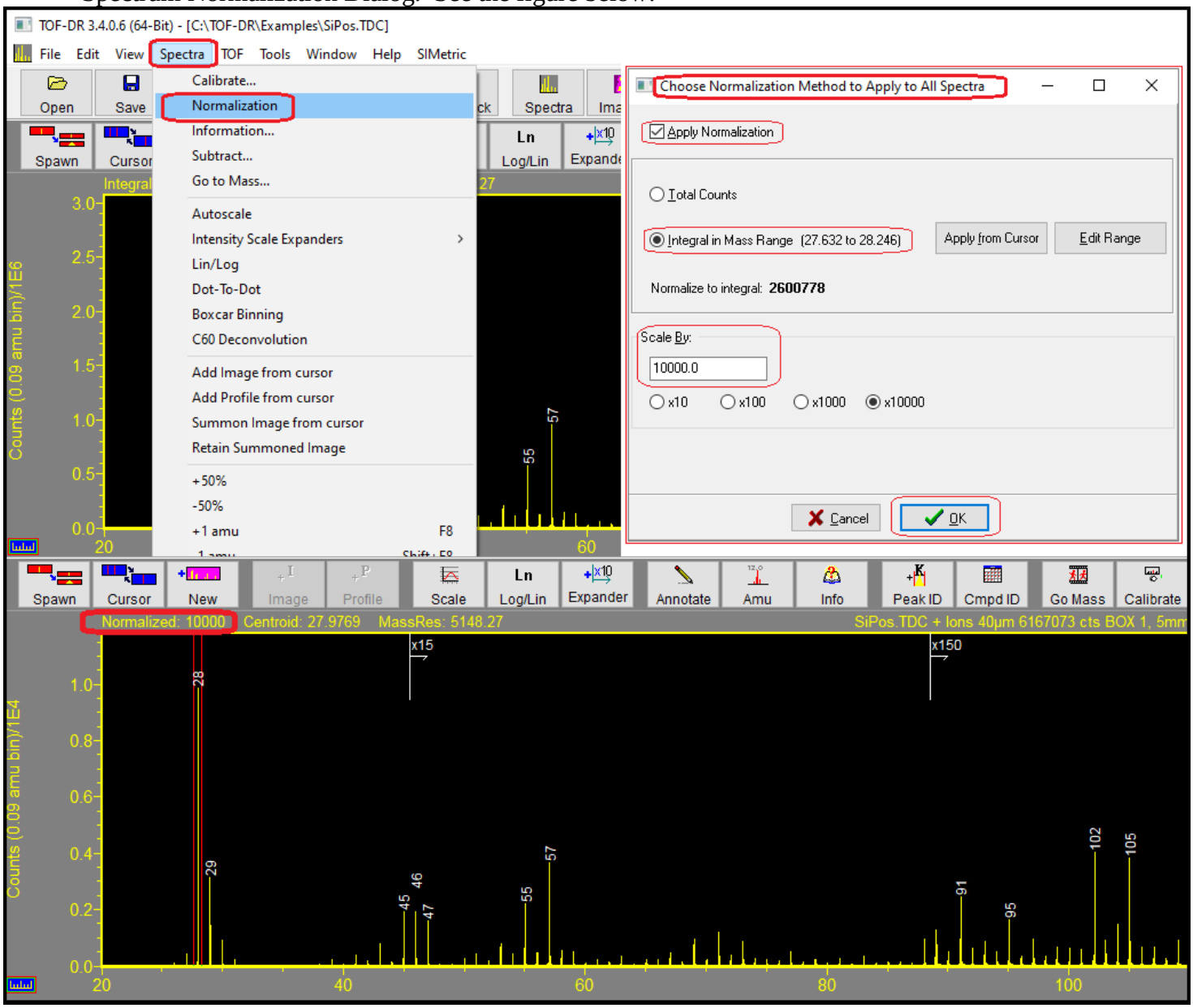


Figure 6 – The Spectrum Normalization Dialog

Within the Spectrum Normalization Dialog. choose a normalization method ('Total Counts' or 'Integral in Mass Range') and a 'Scale By' factor and click OK. Now all the spectra in the Spectrum Window will be normalized by this method. Note that the integral from the double cursor is indicated with the word 'Normalized'.

Note that by clicking the 'Apply from Cursor' button on the dialog, the double cursor mass range (from the current graph in the Spectrum Window) can be applied to the 'Integral in Mass Range' method in order to set the low and high mass (AMU) value.
Also, the mass range can be edited by clicking the 'Edit Range' button.

To turn off this normalization mode, uncheck the 'Apply Normalization' checkbox on the dialog and click OK.

v) Stop Button on Playback UI

A Stop button has been added on the TOFDR playback UI to allow the user a way to abort the playback in progress, if desired.

vi) Image Drift Correction Applied to MSMS Data

In the Image Drift Correction Utility, the Image Drift Correction (which is calculated based on the standard data) is now also applied to MSMS data when the raw data is resaved.

vii) Sputter Beam Alignment Support

In the case where TOF-DR is run in conjunction with SS-TOF for instrument control, sputter beam alignment support has been added to TOF-DR.
On the most recently acquired ion image in the Image Window, right click over the desired feature location and choose the 'Move Sputter Beam to Analysis Beam' option.

viii) Recent Intel Graphics Drivers and the 3D-Image Window

Note: For the problem where the Phi3dViewer error message “Could not obtain OLE control window handle” appears (this problem is specific to computers using Intel® Graphics Driver for Intel® Arc™ Graphics, 11th-13th Gen Intel® Core™ processor graphics), Intel has a new (as of August 2023) driver release that resolves the problem.
On a PC that is experiencing this problem (error message “Could not obtain OLE control window handle”), visit the intel website and download/install version 31.0.101.4577 or later of the Intel® Graphics Driver for Intel® Arc™ Graphics, 11th-13th Gen Intel® Core™ processor graphics.

https://www.intel.com/content/www/us/en/download/726609/intel-arc-iris-xe-graphics-whql-windows.html

Release 3.3.0 – January 2023 (Win10; 64-Bit)

I. Introduction

In this release of TOF-DR, the depth profiling functionality from the SIMetric software package has been added, providing advanced capabilities for examining and displaying profile curve data. This release also includes a number of issues that have been corrected since the release of version 3.2.1.

II. New Features

i) SIMetric Software Package Added

The depth profiling functionality from the SIMetric software package has been added to TOF-DR, providing advanced capabilities for examining and displaying profile curve data.
To display profile date in a SIMetric browser, choose the Open New option from the SIMetric main menu (shown below) and select a data file.

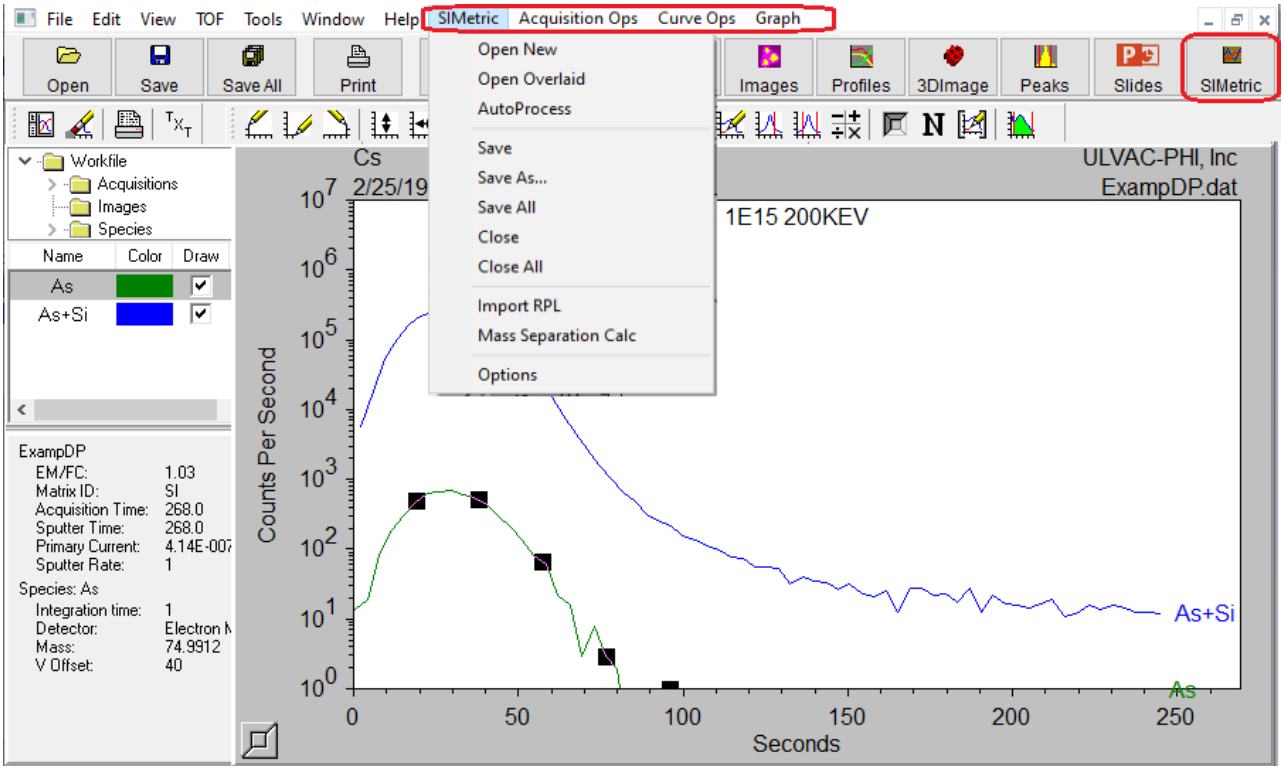


Figure 1 –The SIMetric Main Menu in TOF-DR

Note that this SIMetric capability has been added to TOF-DR without replacing or modifying normal TOF-DR behavior. For example, the TOF-DR Profiles Window remains the default location where profile species curves are displayed after raw data playback.

ii) Raw File Multi-Select

The Raw File Multi-Select feature enables batch-replay including the application of a specified peak file and/or mass calibration file. See the figure below:

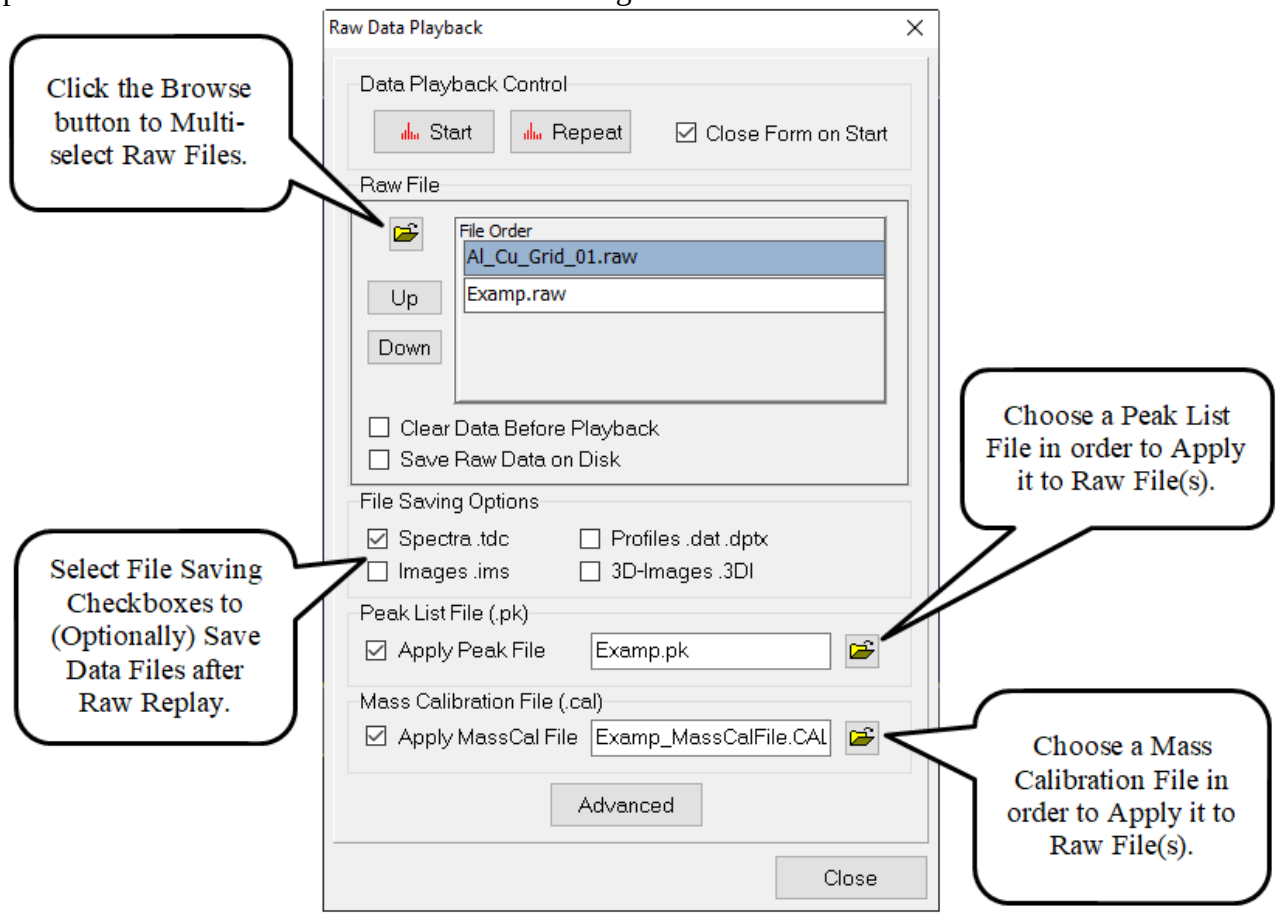


Figure 2 –The Raw Data Playback Form

In other respects, the pre-existing functionality of the form remains available and unchanged. As before, click the Advanced button on this form to see the additional advanced capabilities.

III. Corrected Issues

A. Ion Images from Raw Playback Increased Limit

Increase limit on simultaneously acquiring images for raw playback.

B. Raw Concatenate Utility Widened to Support Long Filenames

The Raw Concatenate Utility form has been widened for long filenames, which will also be shown via the mouse-over hover hint.

C. Restore Calibration Species Mass-sorted in Mass Calibration Form

In earlier versions of TOFDR, the calibration species were sorted by mass by default, which is the proper behavior. This behavior has now been restored.

D. Resolved Error when Importing SSL library

A potential error has been corrected when importing SSL library from the Options form.

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Release 3.2.1 – November 2020 (Win10; 32-Bit)

Release 3.2.1 – November 2020 (Win10; 64-Bit)

I. Introduction

This release includes a number of issues that have been corrected since the release of version 3.2.0.

II. Corrected Issues

E. Up/Down Arrow Behavior Now Consistent in ReviewWin

In ReviewWin, now the Up/Down arrow keypress affects only the Formula (Peak ID) listview (formerly the behavior was inconsistent).

F. Issue with Edit ROI at startup corrected

Resolved an issue with Edit ROI (on the playback UI) when it was invoked immediately after program startup.

G. Improved behavior using the 64bit ACE driver

Improved error handling in situations where the 64bit ACE driver encountered problems.

H. Improved Behavior When Multiple Profiling Peaks Share Name

When multiple profiling peaks share the same name, improve the behavior in the ReviewWin.

I. Improved Logging Behavior During Live Acquire

Avoid unnecessary system log entries during live acquire.

J. Improved Behavior When Acquisition Begins with MassLinked Axes

Resolved an issue where, when an acquistion begins with MassLink turned on in the SpectrumWin, so that the new graph (holding the newly acquiring data) inherits the user's desired mass range.

K. Improved Appearance of TraceMetal UI

Improved appearance of the TraceMetal UI by removing an unnecessary label.

L. Improved Appearance of Axis-label font on Spectra

Axis-label font on Spectra was clipped in some situations.

M. Restored GoMass Capability in the Raw Mass Shift Utility

Restored GoMass Capability in the Raw Mass Shift Utility.

Release 3.2.0 – September 2020 (Win10; 32-Bit)

Release 3.2.0 – September 2020 (Win10; 64-Bit)

I. Introduction

This release includes the redesigned and enhanced Review Window (which replaces the Image Review Tool from previous versions) and a number of other new features and defect corrections.

II. New Features

1 Review Window Redesign and Enhancements

Overview

The Review Window is a dedicated window that allows the user to quickly jump from peak to peak and instantly inspect the peak and corresponding ion image and profile curve from the current acquisition (or most recently replayed raw file). The user can easily identify the peak (choose from a list) and add the peak to the current list of peaks (i.e. the set of peaks seen in the Peak Window). The Review Window also provides a new capability to update/modify an old raw file with a new mass calibration.

Note that the Review Window extends and replaces the Image Review Utility available in earlier versions of TOF-DR.

To launch the Review Window from TOF-DR, first replay a raw file, then click the Review button in the main toolbar (or choose the "Window| Review" main menu option), as shown in the figure below.

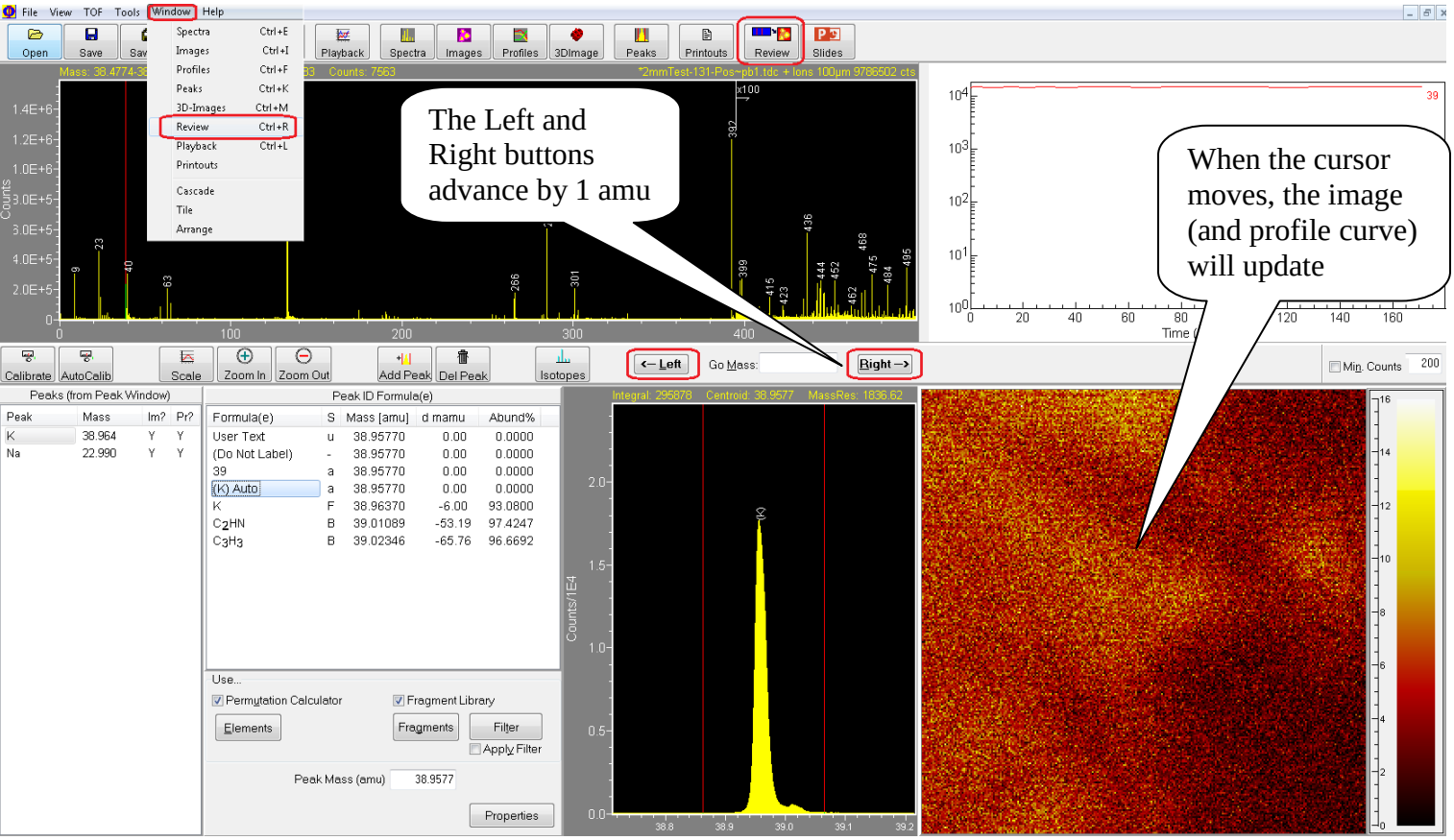


Figure 1 –The Review Window

Adjust the spectrum double cursors and the corresponding image and profile curve 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 the cursor keys (left/right) may also be used).

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

Tools in the Review Window

A number of tools are available in the Review Window (some of which also appear in the Spectrum Window toolbar and function in the same way):

- Calibrate – Mass calibrate the spectrum. Note that the mass calibration utility form now has a new button "Update Raw" that allows the user to update the corresponding raw file with the updated/improved mass calibration for future raw replay.
- AutoCalib – Automatically mass calibrate the spectrum
- Scale – Auto-scale the spectrum graphs and the image color bar
- Zoom In/Out – Contract/Expand the overview (top) graph's mass range
- Add Peak – Add a peak (in the Peak Window) set for imaging & profiling for future acquisitions
- Del Peak – Delete the selected peak from the peak list
- Left/Right – Jump by 1 amu
- Go Mass – Jump to any mass or species
- 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

Review Window During a Live Acquisition

The Review Window 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 Peak Window 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.

Peak ID Capability in Review Window

The Peak-ID capability in the Review Window is very similar in usage to the Pea kid Review Utility Tool from the Spectrum Window. In this way, the user may select from the list of formulae (populated via the fragment library and/or permutation calculator) to explicitly identify and label a peak on the spectrum. Note that the cursor keys (up/down) may also be used to select a formula/option from the list.

Optimization of Raw File Data

In order to implement the Review Window, 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 (and profile) 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.

2 *Update Raw File Mass Calibration*

This version of TOFDR provides a new capability to update/modify an existing raw file with a new mass calibration so that it is automatically applied when the raw file is replayed in the future.

This new feature is accessed from the Review Window by clicking on the Calibrate button on the toolbar. Note that in this case the mass calibration utility form has the new button “Update Raw” that allows the user to update the corresponding raw file with the updated/improved mass calibration. Note that the new mass calibration information will be appended at the end of the corresponding raw file.

3 *Variable Isotope Attenuation Support*

Support for Variable Isotope Attenuation is provided in the Profile Window via the **Profiles |Attenuation Correction** menu option. To apply the correction, first select profile species with non-zero RAF defined, and then click this item to draw a corresponding set of corrected curves.

The correction factor can be set in the Peak Window, in the **RAF** edit box (note that the default value is 0). Note that the specified factor will be saved with the peak objects when the user saves the peak (.pk extension) file. In this way, when the profile objects are created (during a live-acquire or raw replay) the factor (from the corresponding peak) will be passed to the profile objects. And this RAF will be saved with the profile in the profile file (.dat and .dptx).
(Note: in order to apply these factors to profile data collected via older software versions, you can add/edit the RAF in the .dptx file, and then open that file in TOFDR).

4 *Image Window Swap File with Spectrum Column Header*

In the Image Window listview right-click popup-menu, a new option has been added a "Swap File / Spectrum Column Header". The listview’s includes a File column by default, but in cases where multiple sets of data are saved into the same .imps file, it can be preferable to see the images corresponding Spectrum name in order to differentiate datasets. This menu option allows the user to toggle between these as desired.

III. Defects Corrected

A. Improved Behavior for Stay-On-Top Forms

Some Stay-On-Top forms, such as the Playback and Slide Preview etc. should now demonstrate an improved behavior when other applications are activated or appear on top of TOFDR – these forms should now be visible only when the TOF-DR UI is visible.

B. Improved Behavior after Cancel on Spectrum Save

Resolved an issue with spectrum save when, after user clicks cancel in the info (comment) dialog, TOF-DR should cancel the save operation.

C. Correct Mass-Linked Axes Behavior after GoMass

Mass-Linked axes now behave properly (formerly failed) after using GoMass in the Spectrum Window.

D. Improved Delete Behavior after New in Spectrum Window

Resolved an issue after New tool-button click (on a spectrum), where Delete caused problems in the Spectrum Window.

E. Support Legacy Raw Files Containing Pulsed SED Image Data

Improved behavior where, if SEM data is detected in older raw files (e.g. RawFileFormatVersion = 3.0 files created by WinCadenceN), TOF-DR will try to show the SEM image even when the corresponding raw file ASCII header tag is missing.

F. Batch Auto-Calibrate Succeeds

Improved behavior in Trace Metals and Organics Report Generation so that auto calibrate the batch succeeds.

G. Improved Behavior in the Mass Calibrate Form

Improved behavior in the Mass Calibrate Form where formerly when the user pressed the <Enter> key after editing a calibration species, then clicked ‘Add Peak to Calib List’, TOF-DR would display an erroneous warning prompt in some cases.

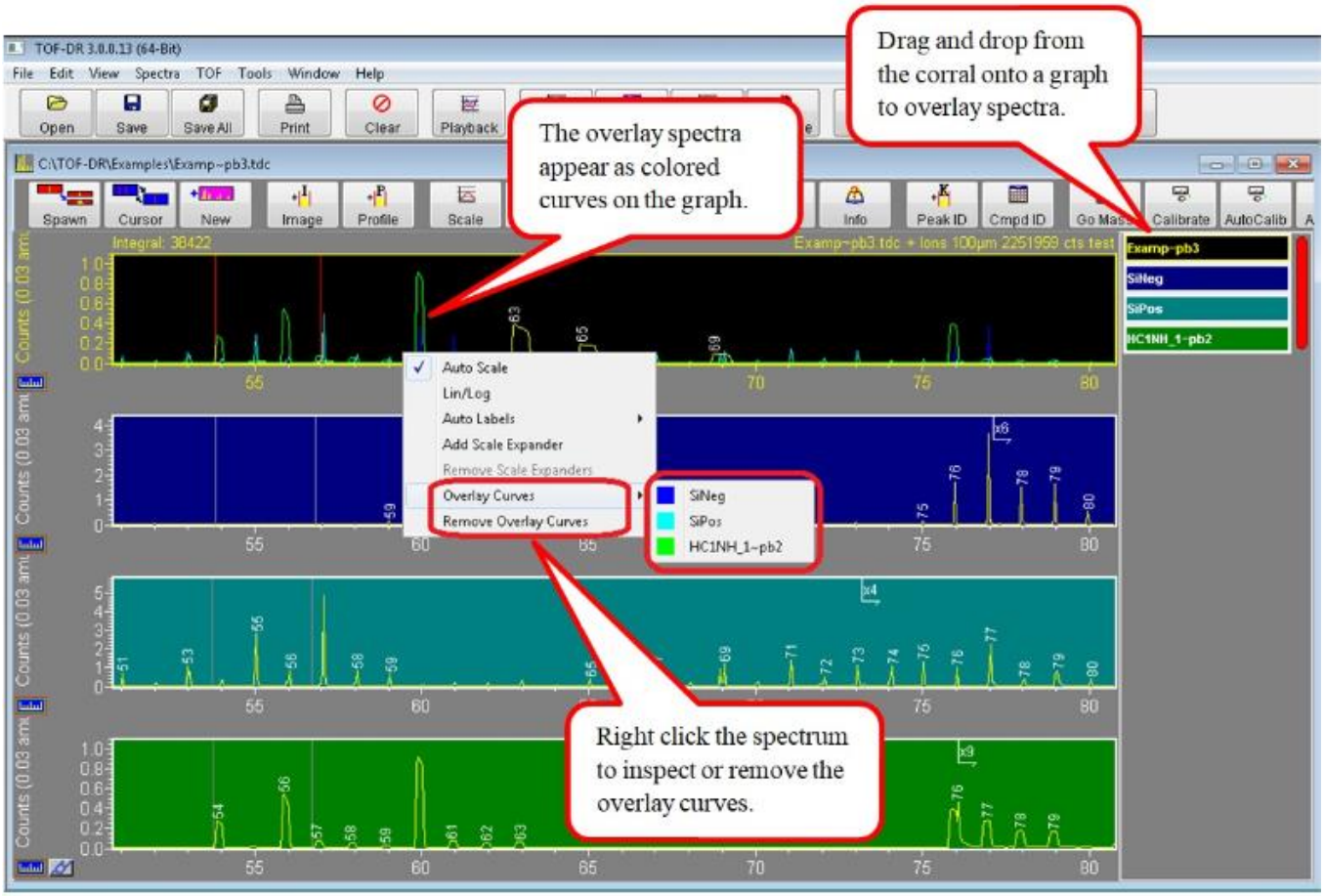
Release 3.1.0 – September 2019 (Win7/Win10; 32-Bit)
Release 3.1.0 – September 2019 (Win7/Win10; 64-Bit)

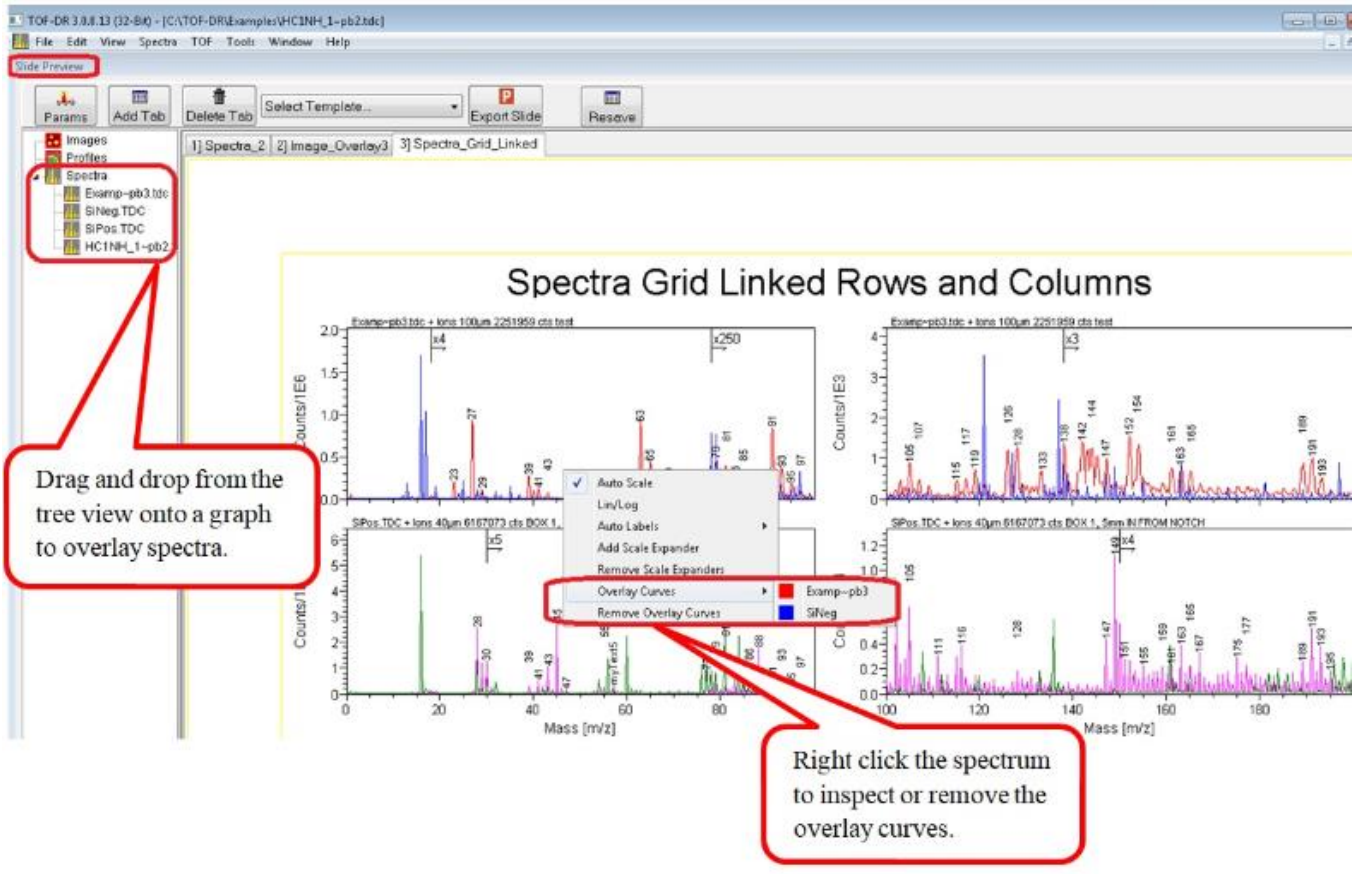
I. Introduction

This release includes defect corrections and a number of new features, including Spectrum Overlay as well as Region Of Interest (ROI) features and extensions.

II. New Features

1 *Spectrum Overlay*





2 ROI (Region of Interest) Features and Extensions

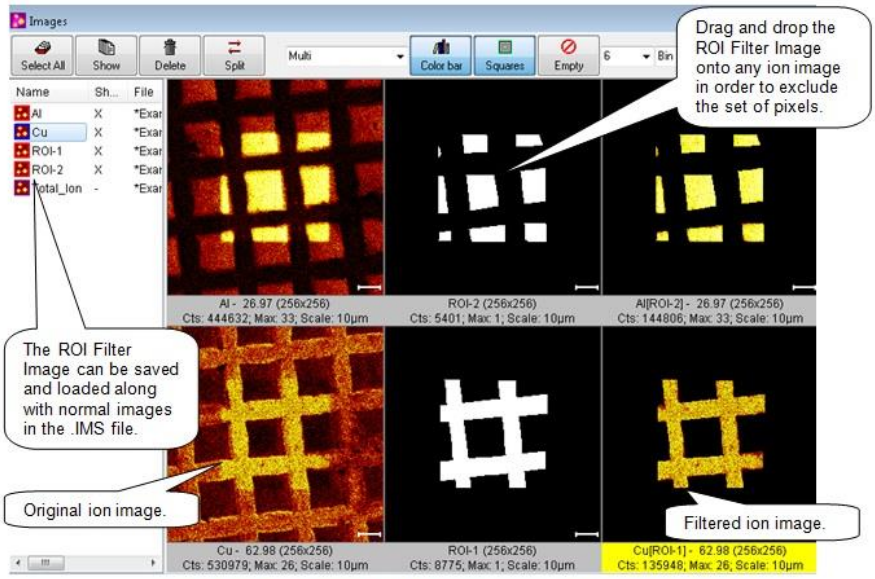


Figure 1 –ROI-Filter Images and filtered ion images in the Image Window

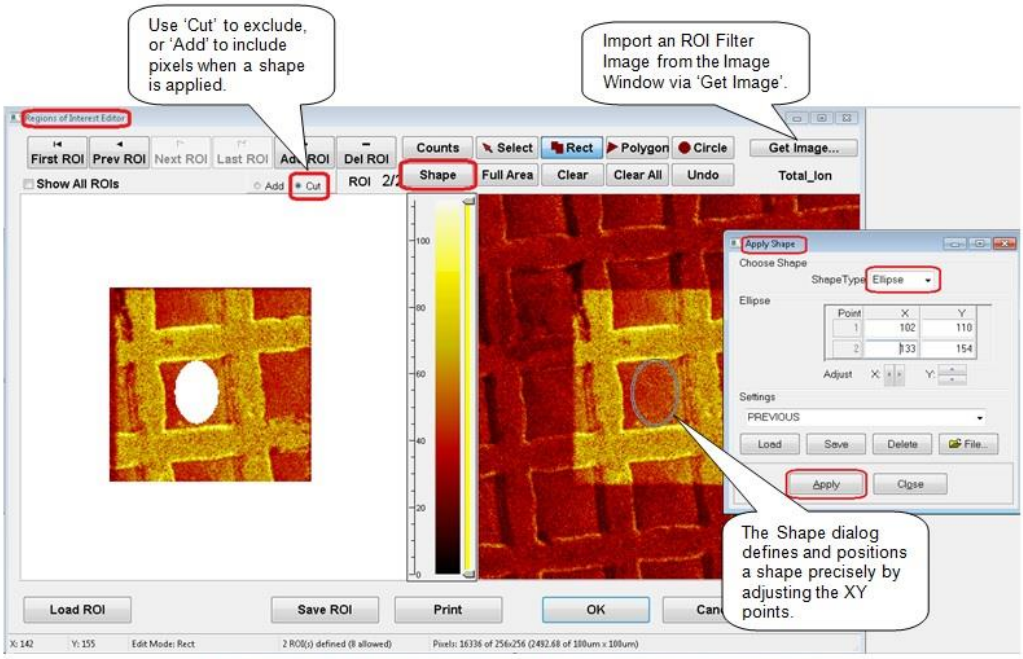


Figure 2 – The ROI Editor and the Shape Dialog for defining a shape precisely.

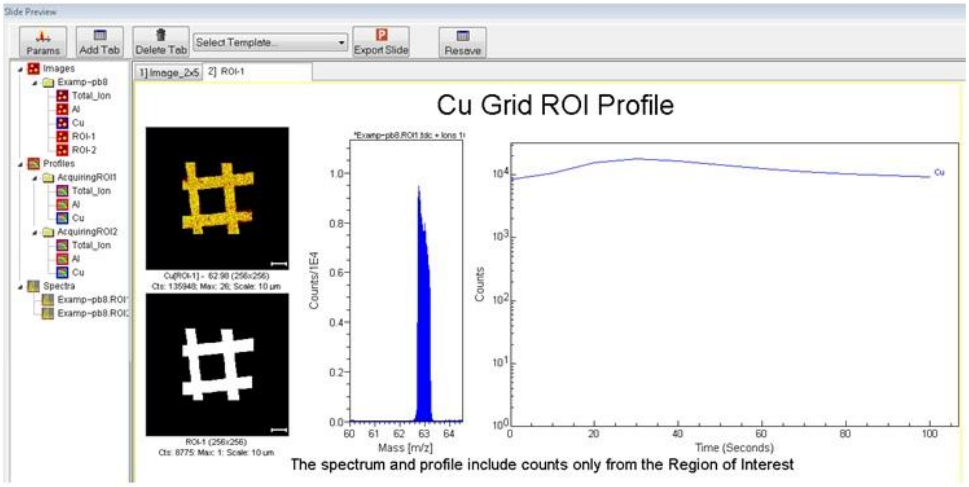
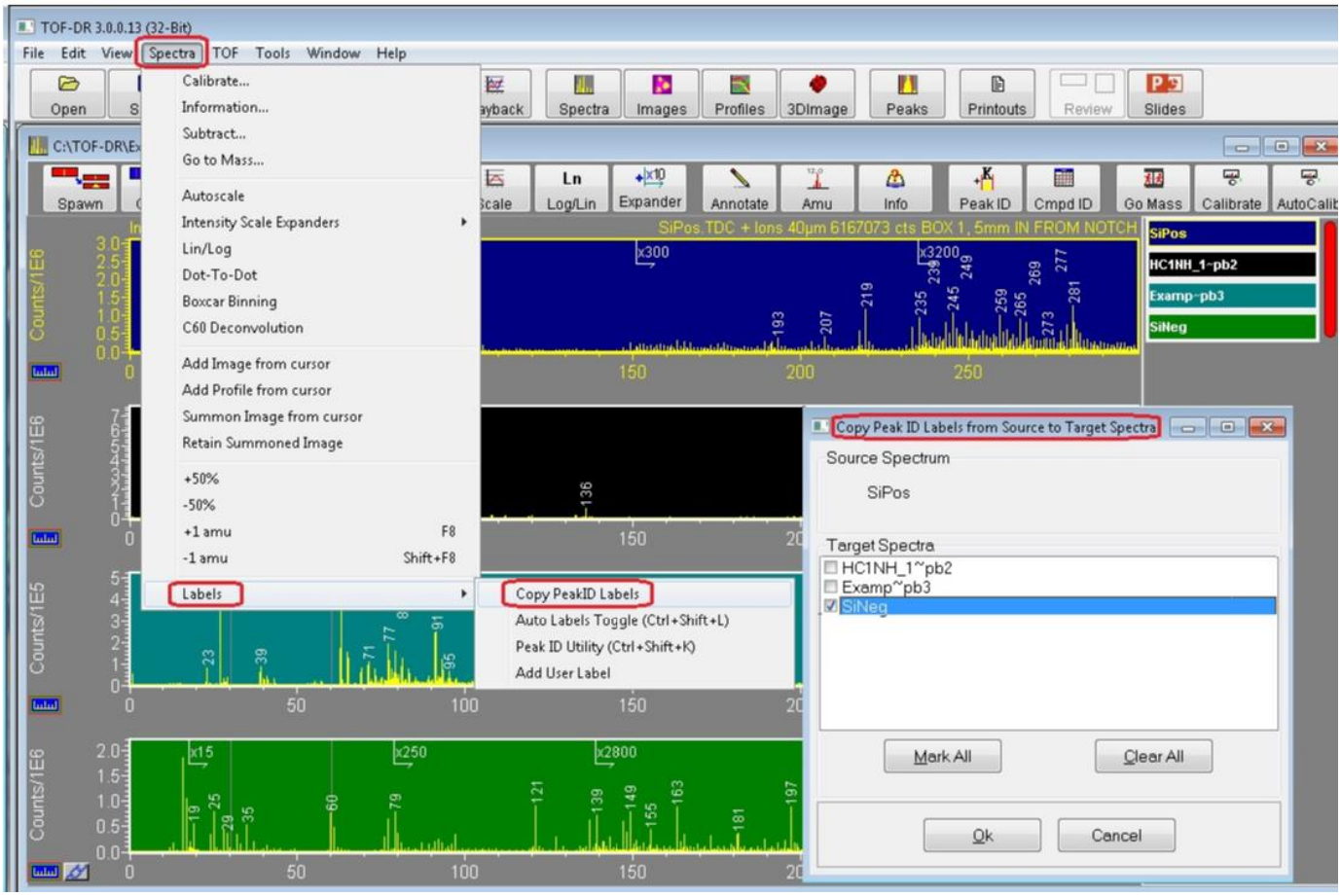


Figure 3 – The Slide Preview Window displaying ROI data.

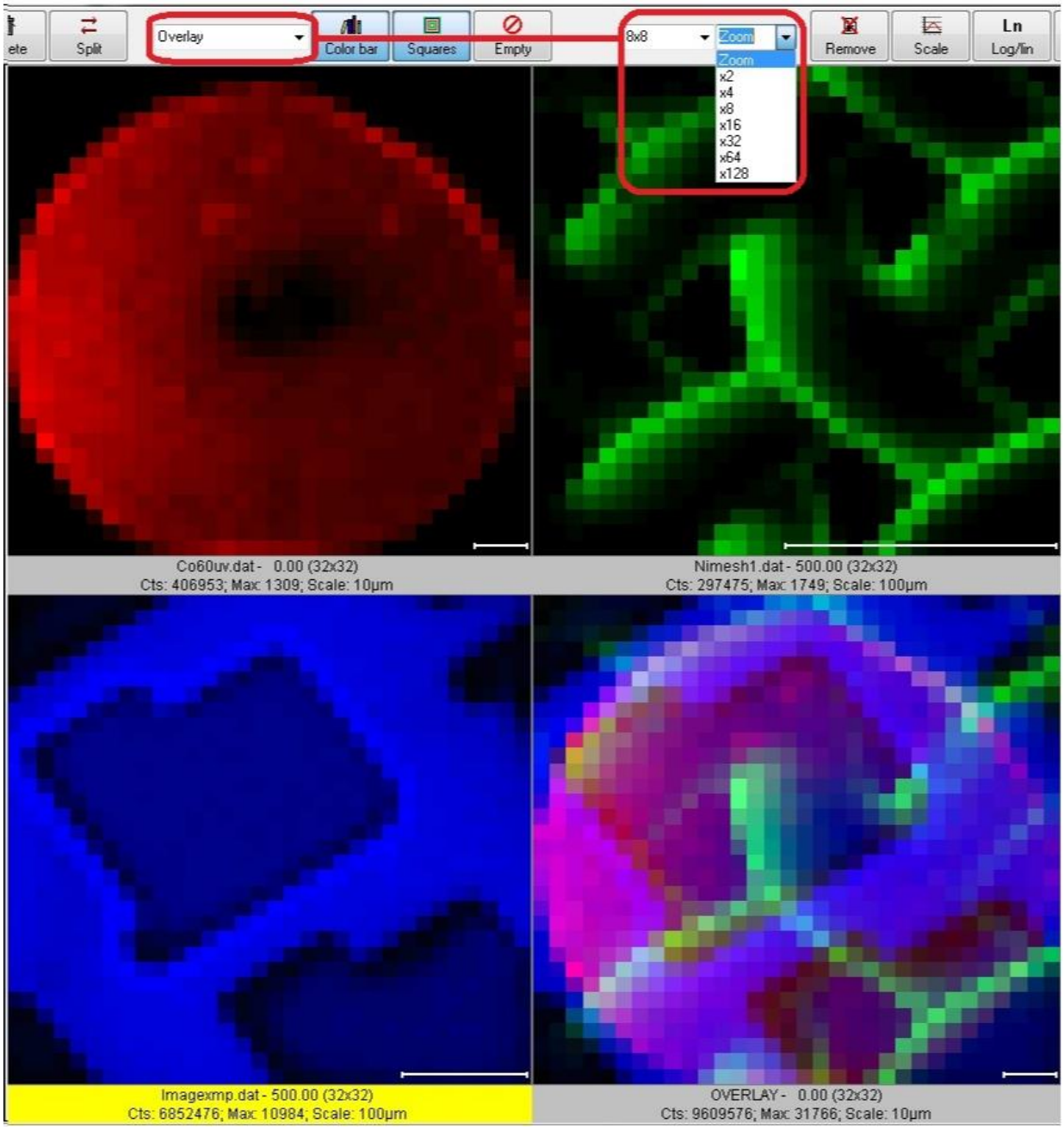
3 *Copy PeakID labels to Target Spectrum (from Source spectrum)*



And note that this feature can also be used to <u>remove</u> labels from the target spectra (if the source spectrum has none).

4 *Three Color Image Overlay Zoom and Bin*

Zoom and Bin Support for the 3-color image overlay feature



5 *Apply User's Spectrum Mass Range from Prior Acquisition*

For the new acquisition's graph in the Spectrum Window, apply the user's spectrum mass range from the prior acquisition.

---

6 *Resave Toolbar Button on Slide Preview*

The Resave toolbar button on the Slide Preview allows user to resave the Template with the current configuration of graphs mass ranges, labels etc.

---

7 *AMU labels optionally drawn horizontally (or vertically)*

Added option to draw AMU-Labels horizontally (not vertically) as was done in prior versions. See the 'AMU-Labels Vertical' checkbox in the Tools|Options|GraphPresentation dialog.

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8 *Profile Graph Axis-Range context menu*

For Profile graphs in the Profile Window and Slide Preview, a mouse right-click on a graph-axis now will pop up the context menu to adjust the axis range lin/log etc. (in the same way as is done for Spectrum graphs) for both X and Y.

---

9 *Faster Slide Preview Export*

In the Slide Preview, the “PPT export” is now faster. [Graph drawing speed has been improved by a factor of 3x.]

---

10 *Copy to clipboard button in ROI editor*

In the ROI editor, a new “Copy” toolbar button has been added to copy the ROI image (as a bitmap) to the Windows clipboard.

---

11 *New Text-based depth profile file format (.DPTX)*

Saves/loads all profile data (including Normal and MSMS data as well as all ROI data) from an acquisition (or raw playback). The .dptx file will be saved automatically and additionally whenever the save of profile data is performed. To load the .dptx file, choose the .dptx file type in the file type dropdown of the data load dialog.

---

12 *Add 'Empty' tool button to the Slide Preview toolbar*

When the Empty tool button is clicked, all data in all viewers of the current slide will be removed.

---

13 *Add CopyToClipboard Tool button to Slide Preview tool bar*

Places the bitmap on the clipboard.

14 *The AcqStatus Dialog is no longer shown during Raw file playback*

The dialog (which was Stay-On-Top) will not be shown during Raw file playback (i.e. it is no longer ‘always on top’ of other applications during playback). Instead now a progress bar appears on the Main Window status bar.

---

15 *Profile Graph Shows XY Value as Hint Text on Status Bar*

On profile graphs- the x and y values of a data point are shown on the status bar when the mouse hovers over the data.

---

16 *Calibrate tool button added to Peak Window*

The Mass Calibrate tool button was added to the Peak Window toolbar.

III. Defects Corrected

A. Automatic Data Save

Automatic Data Save -- when requested by SS-TOF (and also via the SaveAll toolbar button in TOF-DR) will now save all spectra, profiles, and images associated with the current acquisition, including MS2 spectra, profiles, & images, and all ROI spectra, profiles, and Images.

B. Correct Residual Display Detritus after Slide Preview ExportToPPT

Clean up residual spectrum name etc after Slide Preview ExportToPPT

C. Correct the X range when LineScan Toggle Projection is changed

Ensure that the X range is updated properly when the LineScan Toggle Projection changes the range of the selected linescan.

D. Add Compound in Compound ID Corrected

Add Compound in Compound ID Corrected to avoid an error message that appeared in some circumstances.

E. Corrected PeakID Behavior

In PeakID, corrected a problem with rapid repeat of Left-Arrow or Right-Arrow key, which could alter existing labels unpredictably.

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 ‘∑’ 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)

1. Introduction

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

2. New Features

a) Native 64bit support -- TOF-DR is now available as a native 64bit application within 64bit versions of MS Windows.
b) 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.
c) 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.
d) 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.
e) 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.
f) 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).
g) 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.
h) 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.
i) 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.
j) 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.
k) 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.
l) Allow user to modify the linescan averaging width from a right-click popup menu on the linescan viewer in the image window.
m) 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.
n) 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.
o) Extended the playback UI time window limit feature so that the user may optionally define a cycle range window.

3. Defects Corrected

a) Save subtracted spectra to .tdc file now saves properly.
b) The Image Inspector Cursor Info now updates properly on the right side in the cursor area.
c) 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.
d) 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.
e) 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

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.

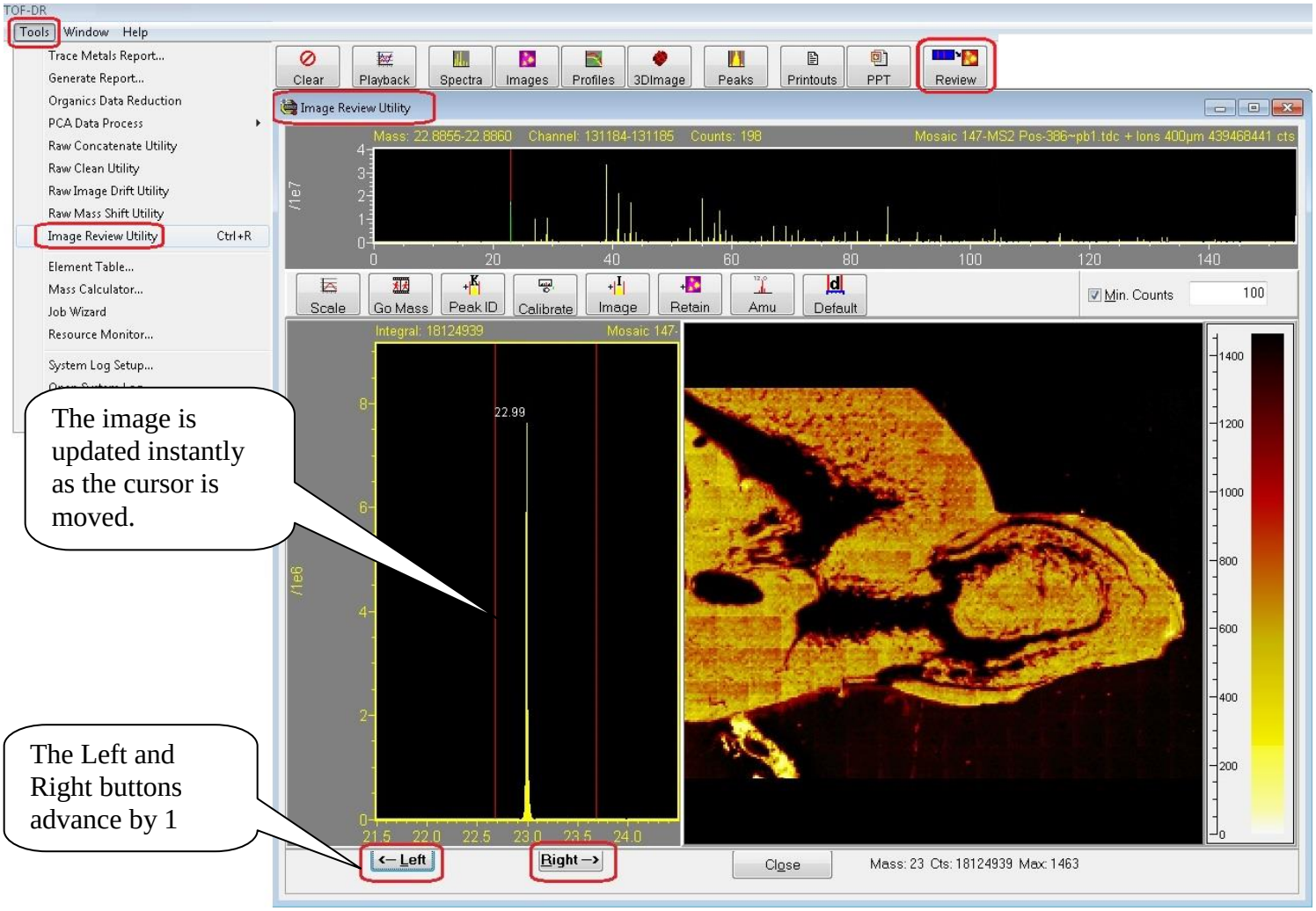

Figure 1 –The image Review Utility

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

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.

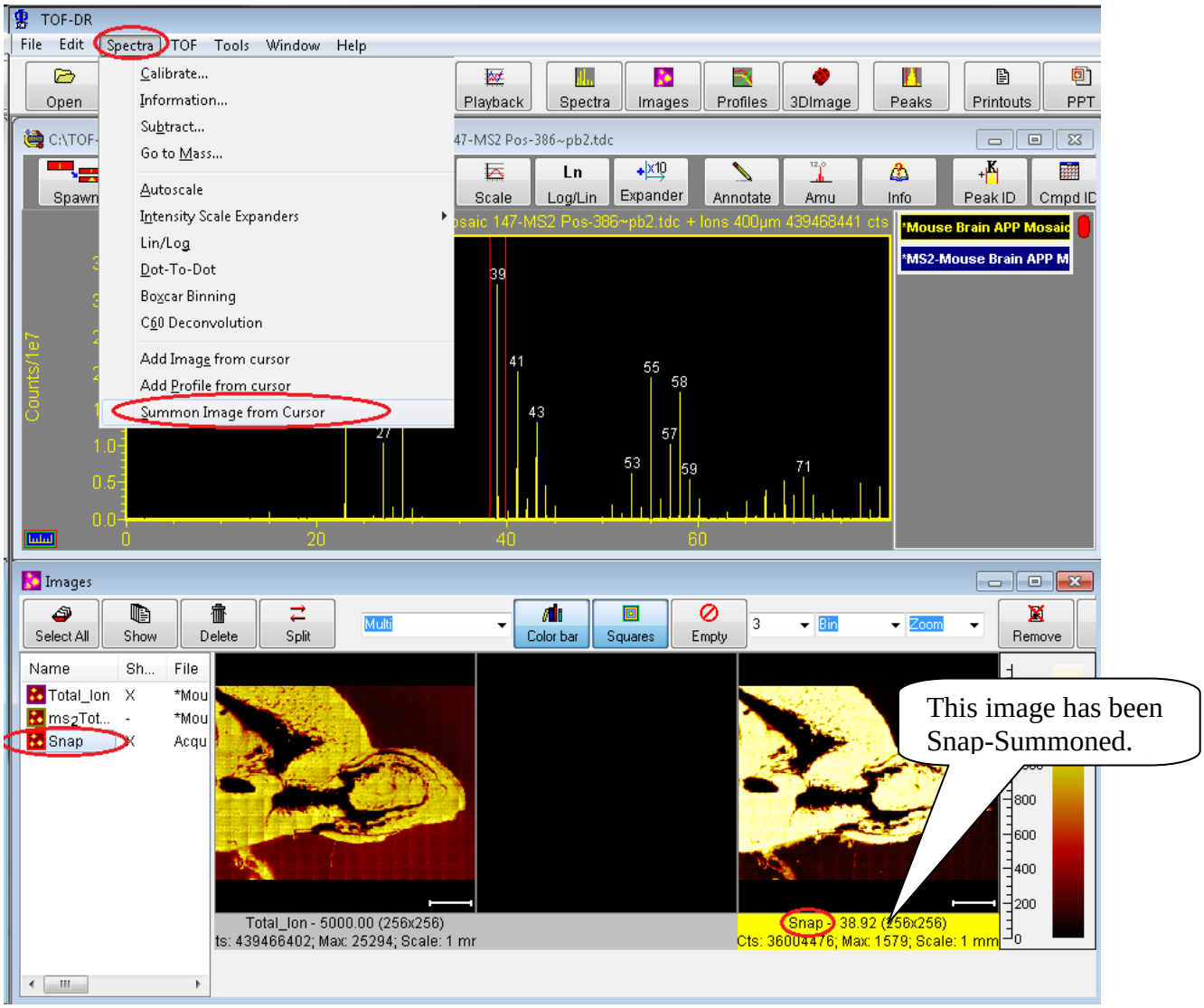

Figure 1 – An ion image has been 'Snap-Summoned' to appear in the Image Window.

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.

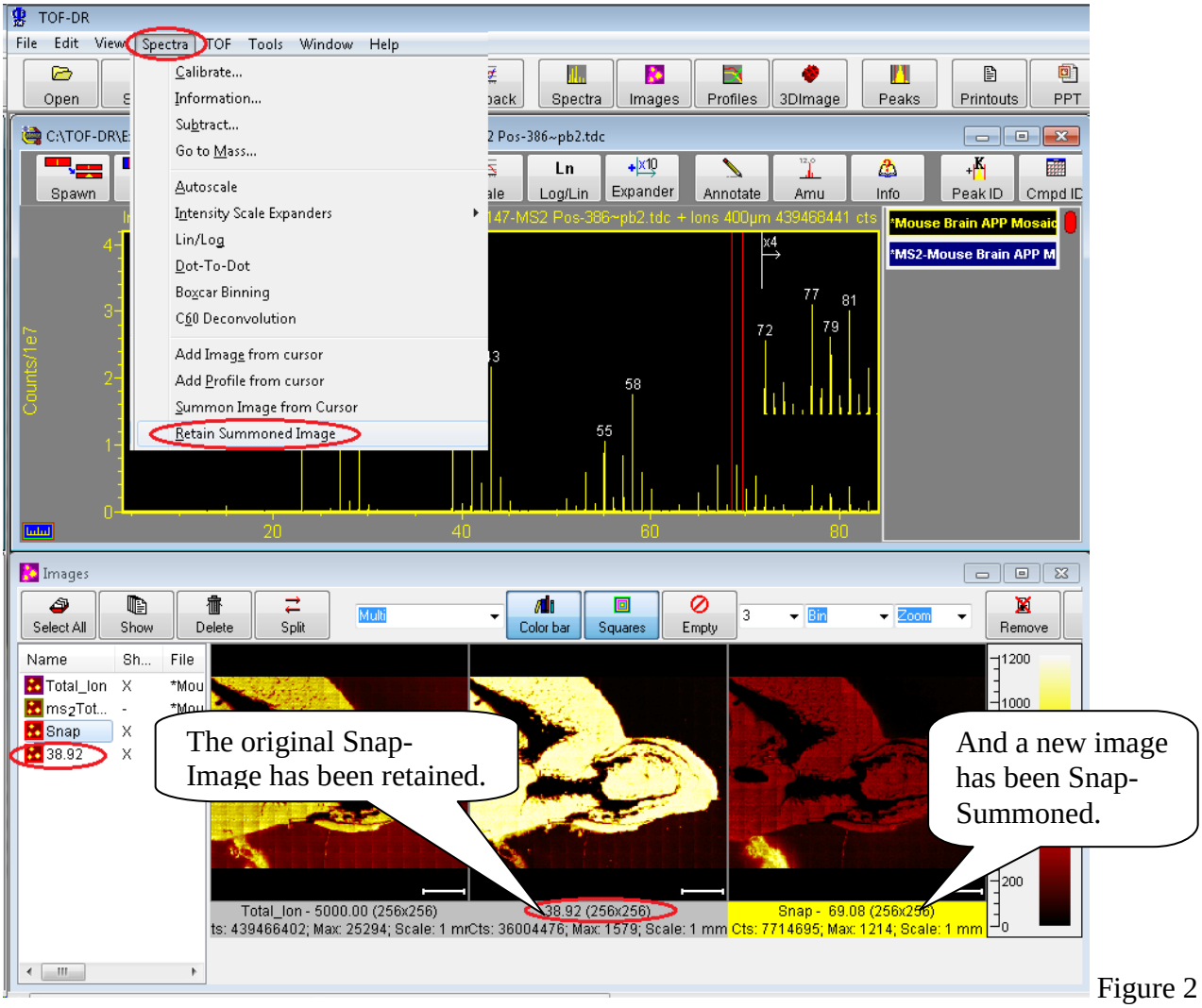

Figure 2 – The original Snap-Image has been retained.

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.

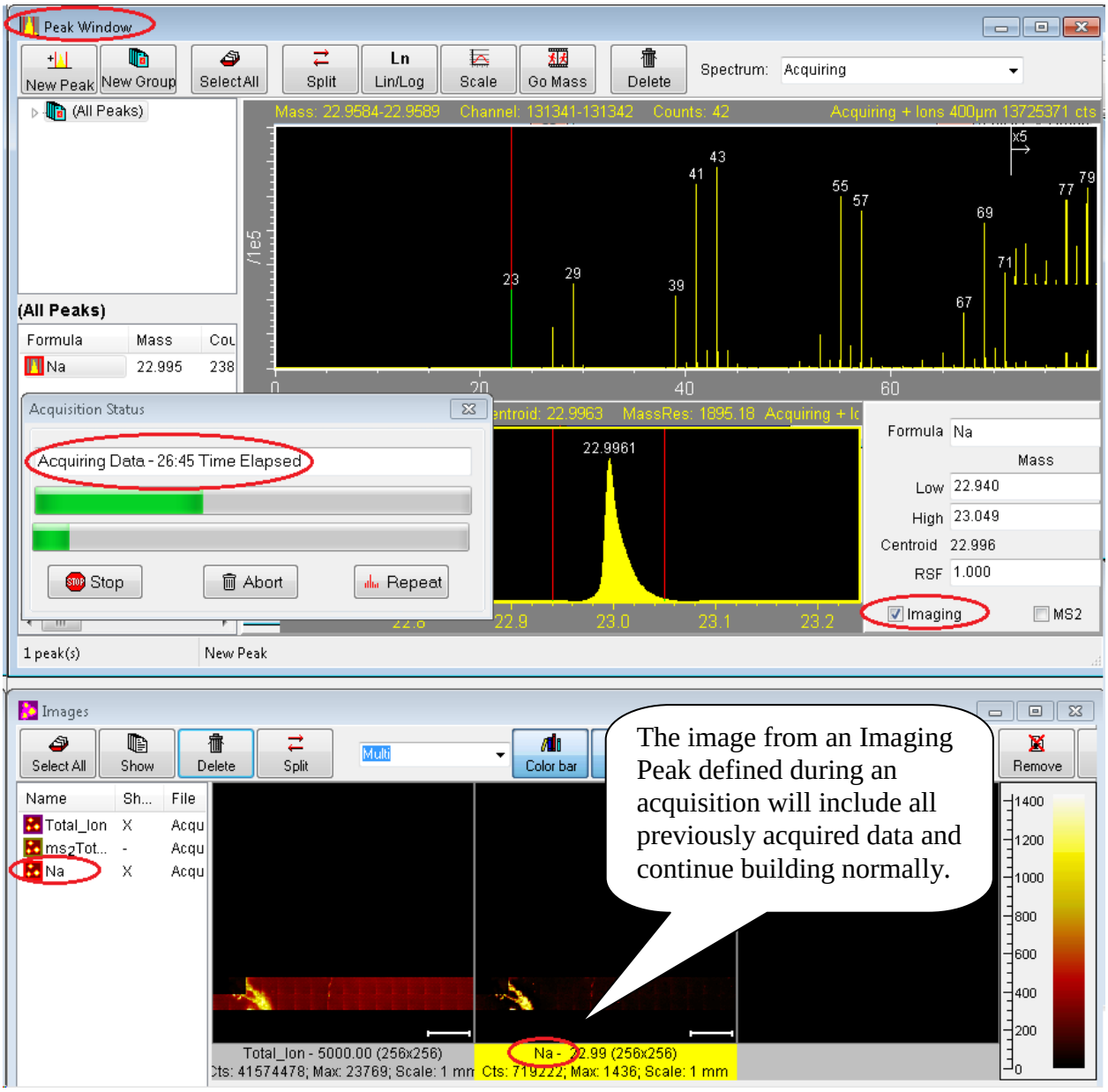

Figure 3 – The image from an Imaging Peak defined mid-acquisition will show all previously acquired data.

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

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.

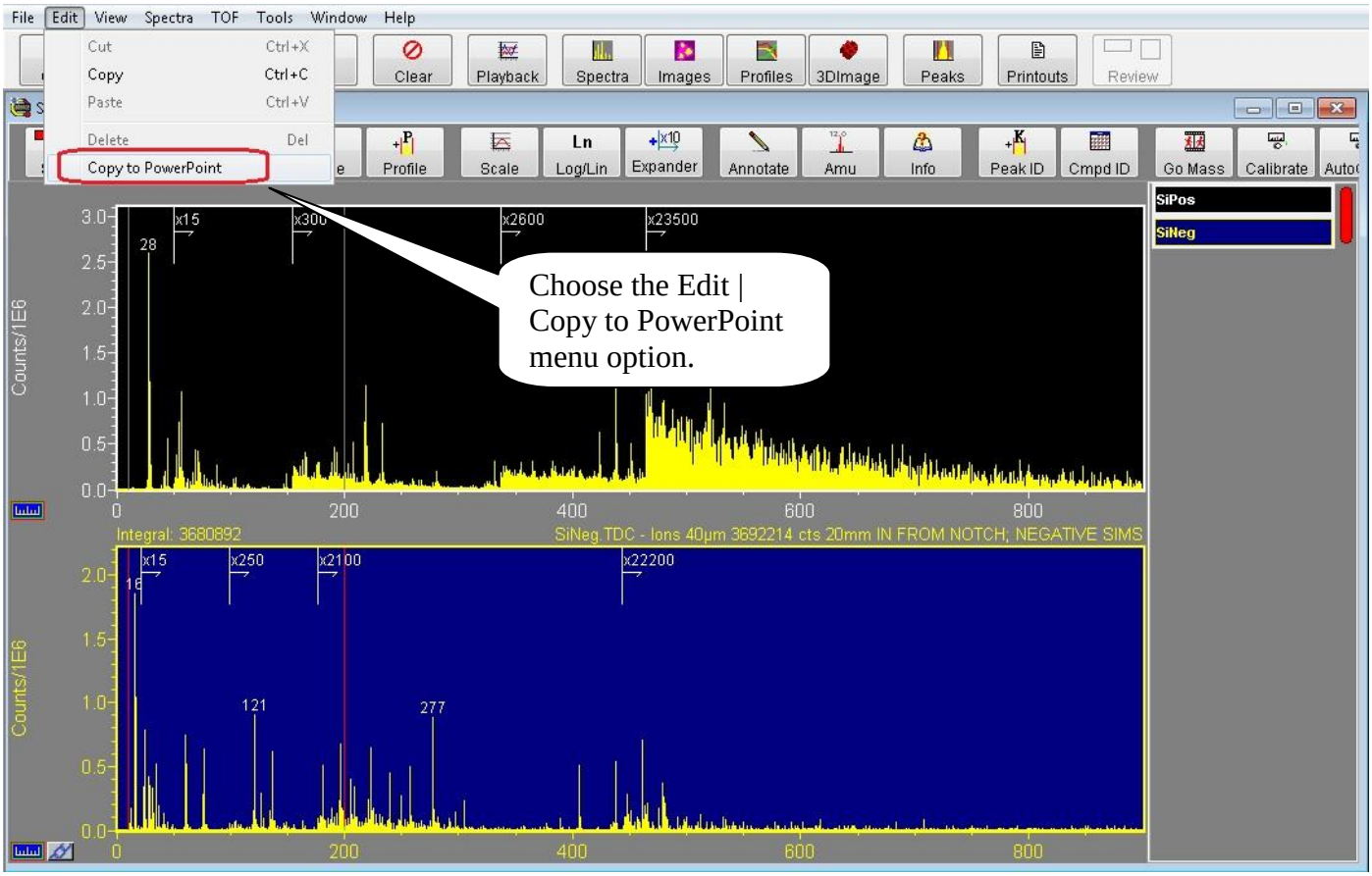

Figure 1 – Spectrum Window Edit | Copy to PowerPoint menu option

The Export to PowerPoint dialog will appear as shown below

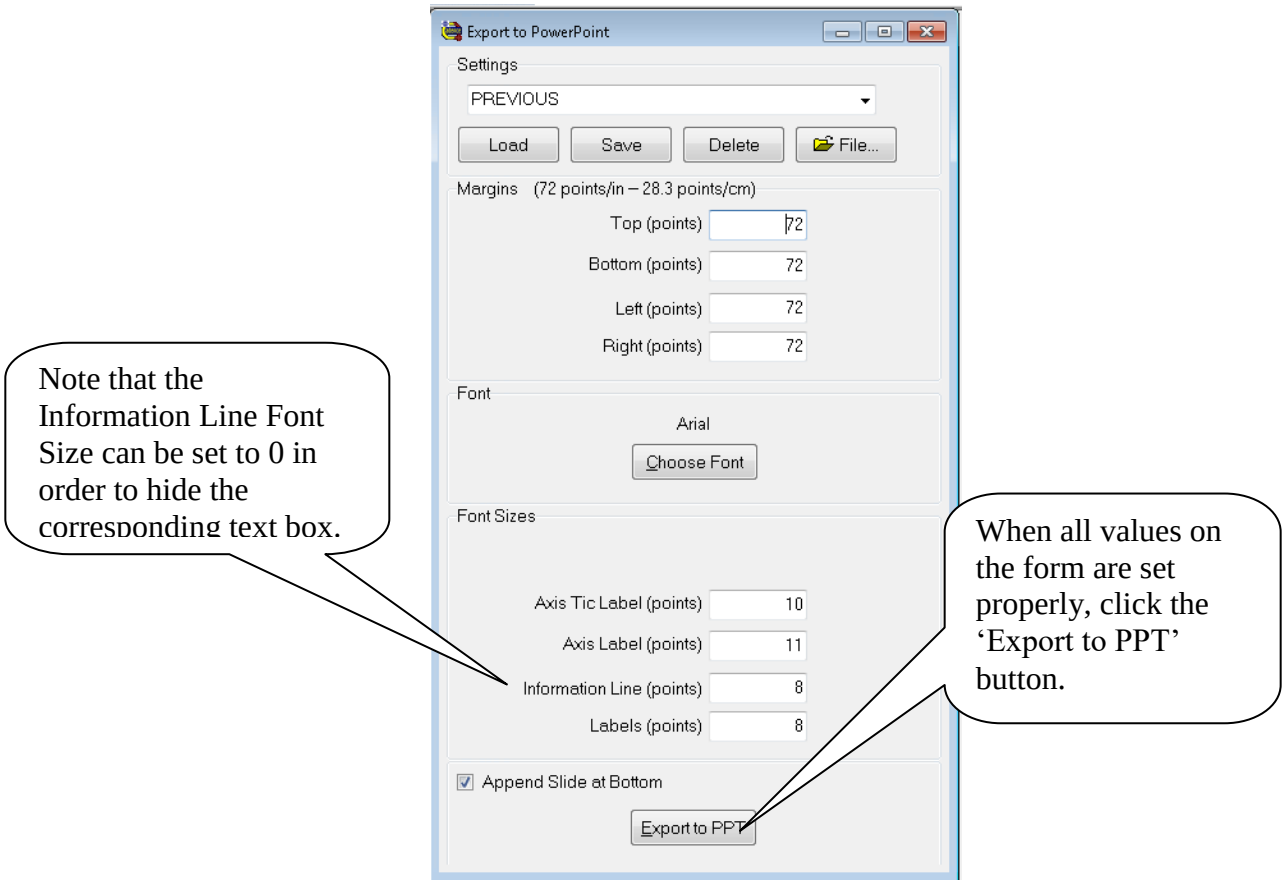

Figure 2 – The Export to PowerPoint dialog

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.

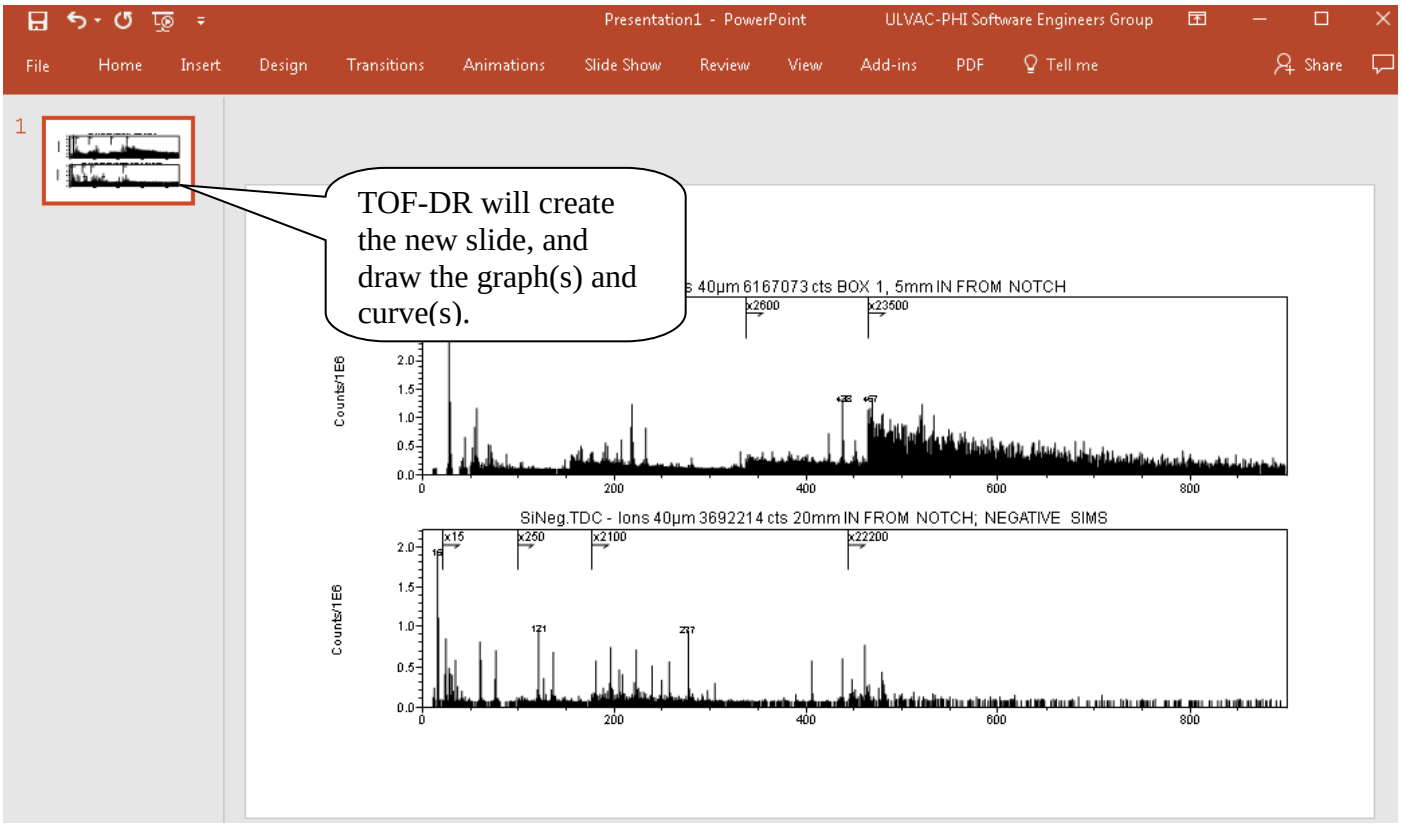

Figure 3 – The Newly Created Slide in PowerPoint

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.

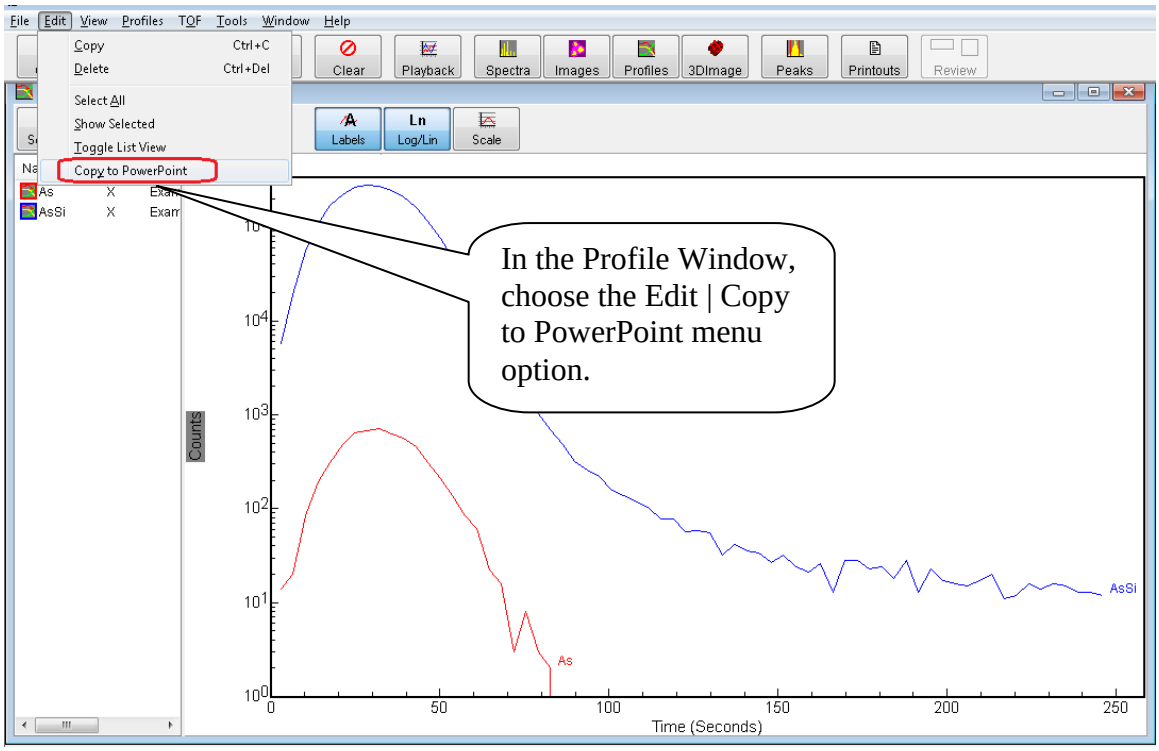

Figure 4 – Profile Window Edit | Copy to PowerPoint menu option

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.

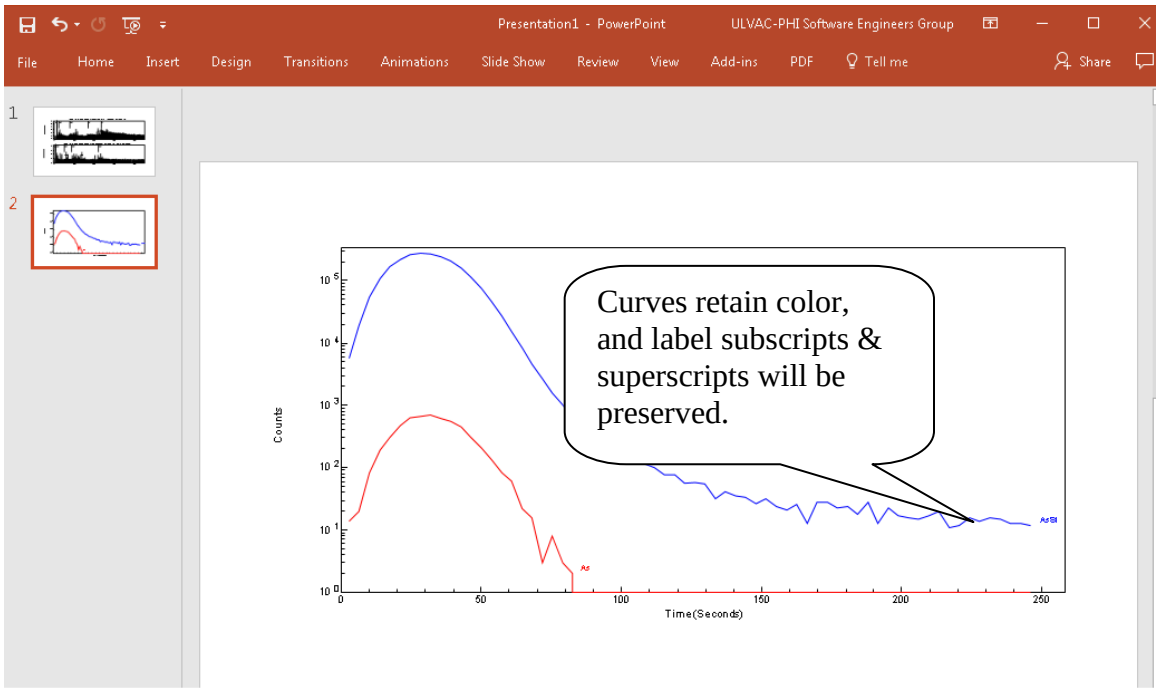

Figure 5 – The Newly Created Slide in PowerPoint

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.

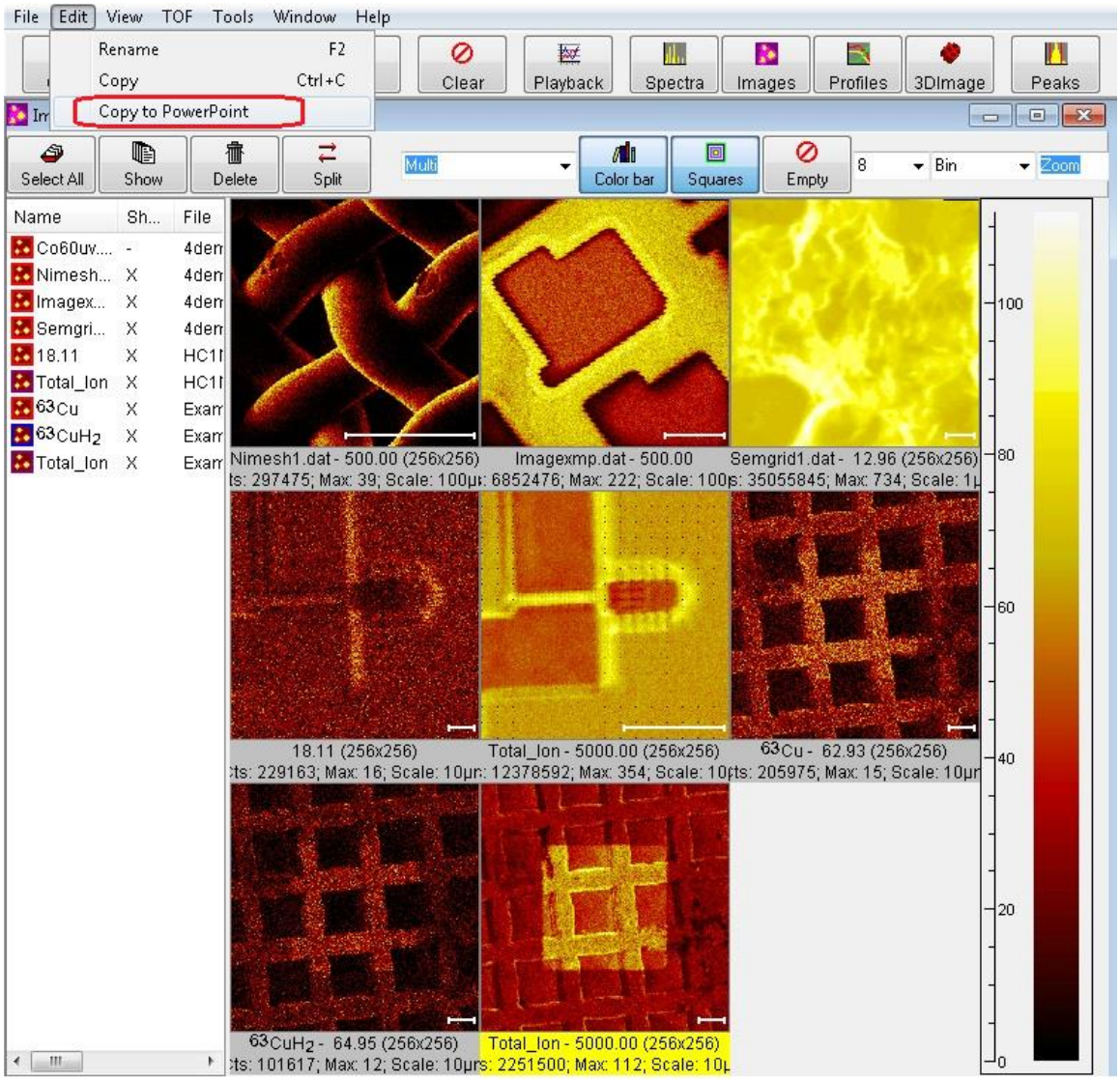

Figure 6 – Image Window Edit | Copy to PowerPoint menu option

The Export to PowerPoint dialog will appear as shown below.

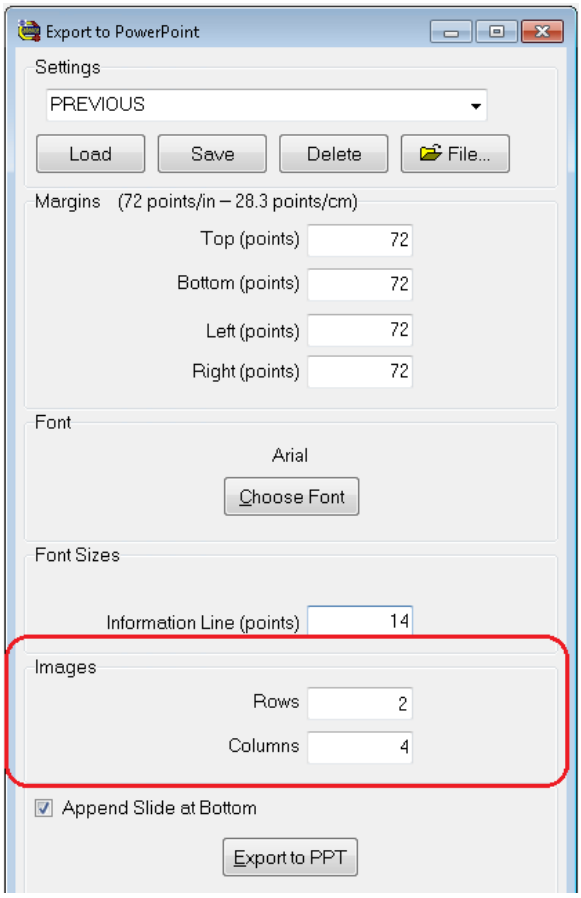

Figure 7 – The Export to PowerPoint dialog with Image Rows and Columns

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.

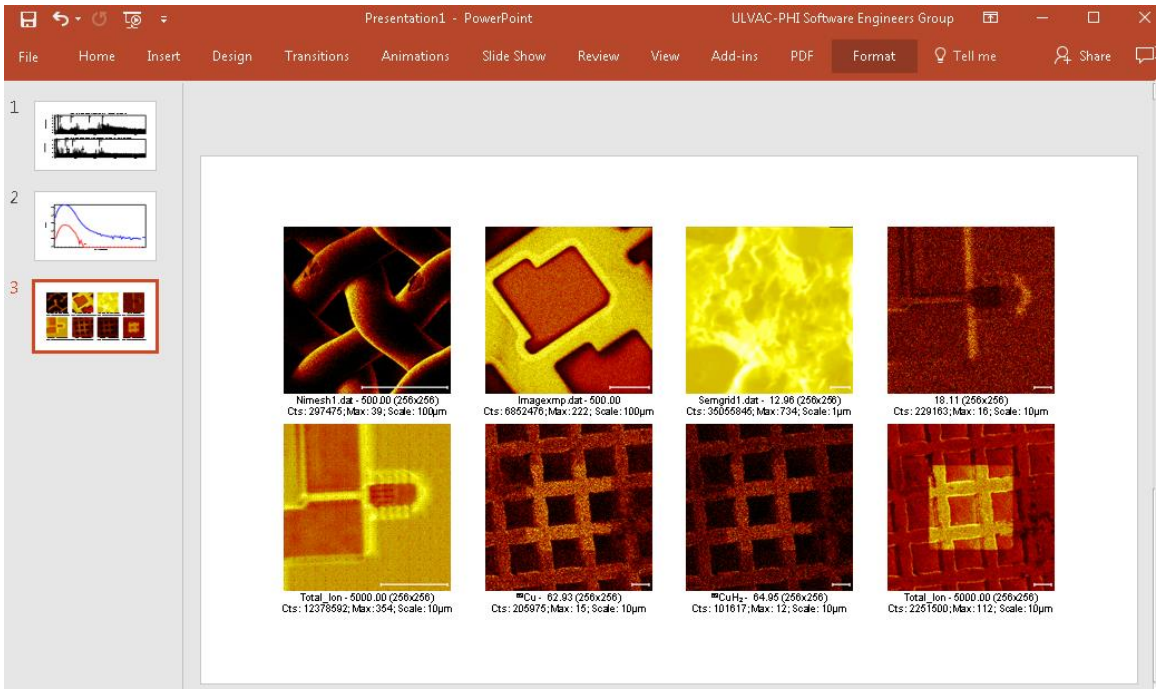

Figure 8 – The Newly Created Slide in PowerPoint

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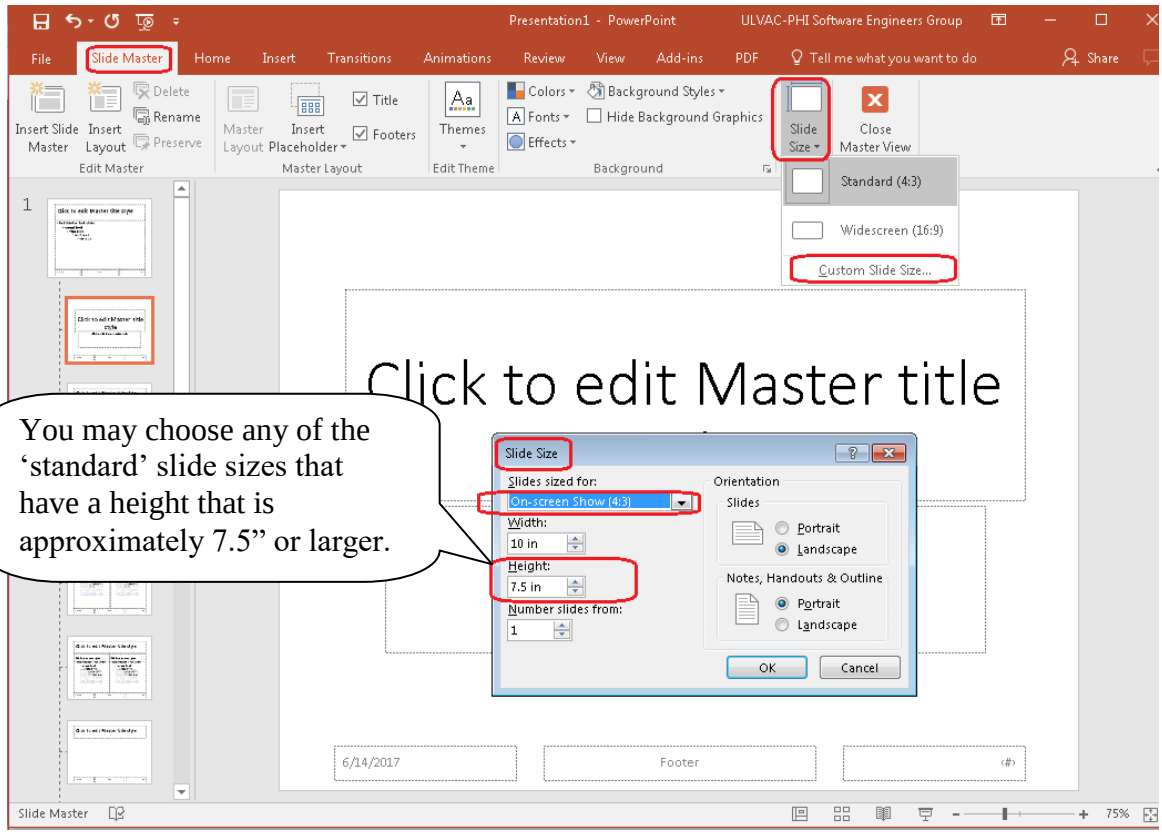
Important Note – Master Slide Height in PowerPoint

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

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.

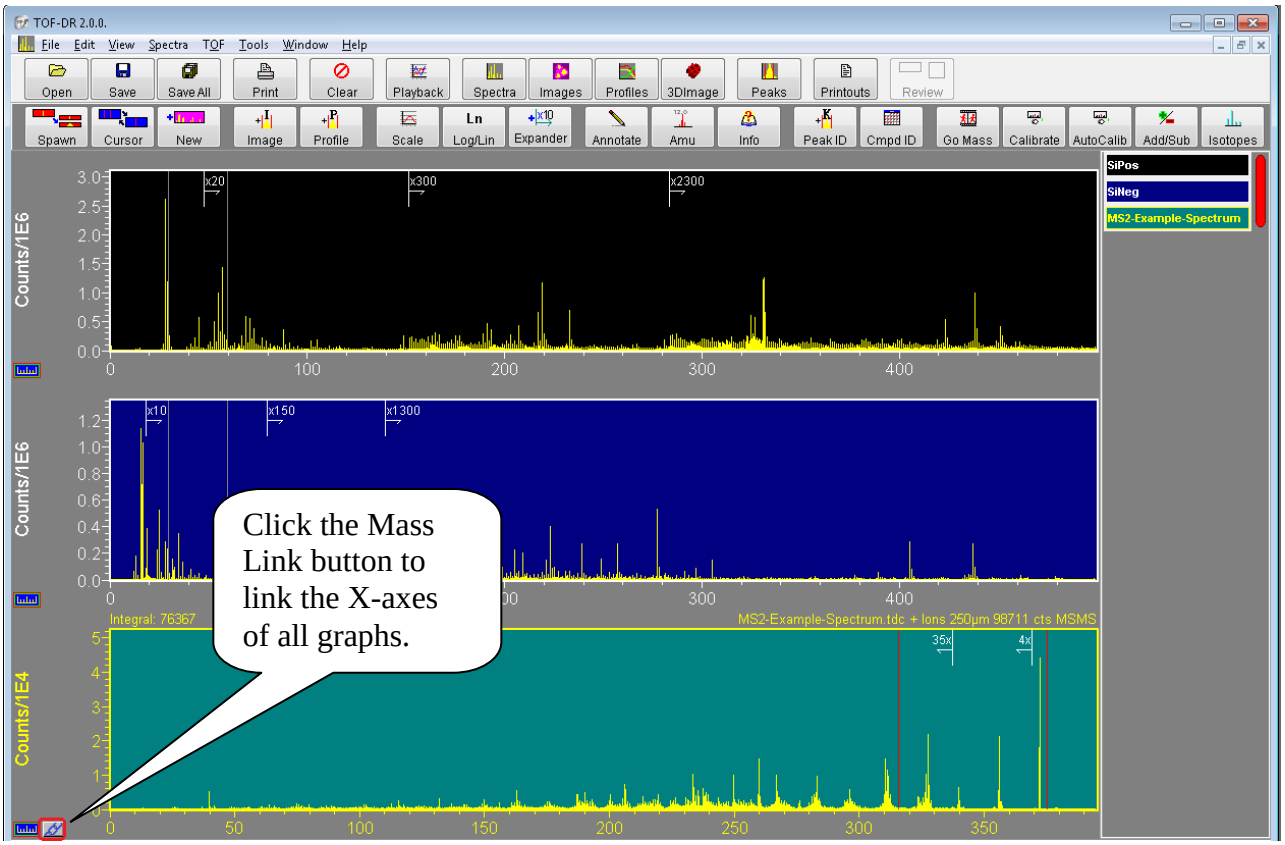


Figure 1 – Click the Mass Link button to link the X-axes

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.

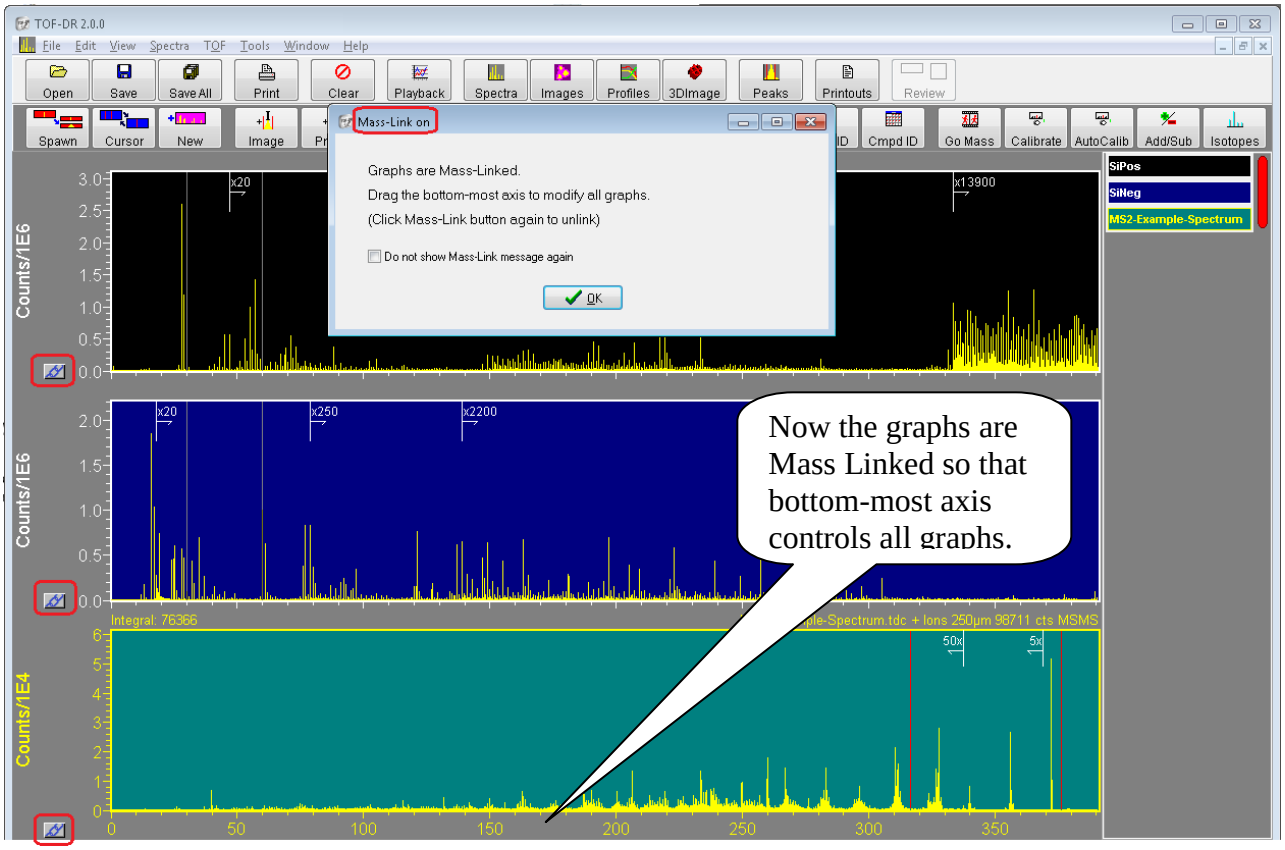


Figure 2 – The Graphs are Mass Linked

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.

I. Release 1.4.0 – October 2016

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

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

TOF-DR Version 1.4

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.

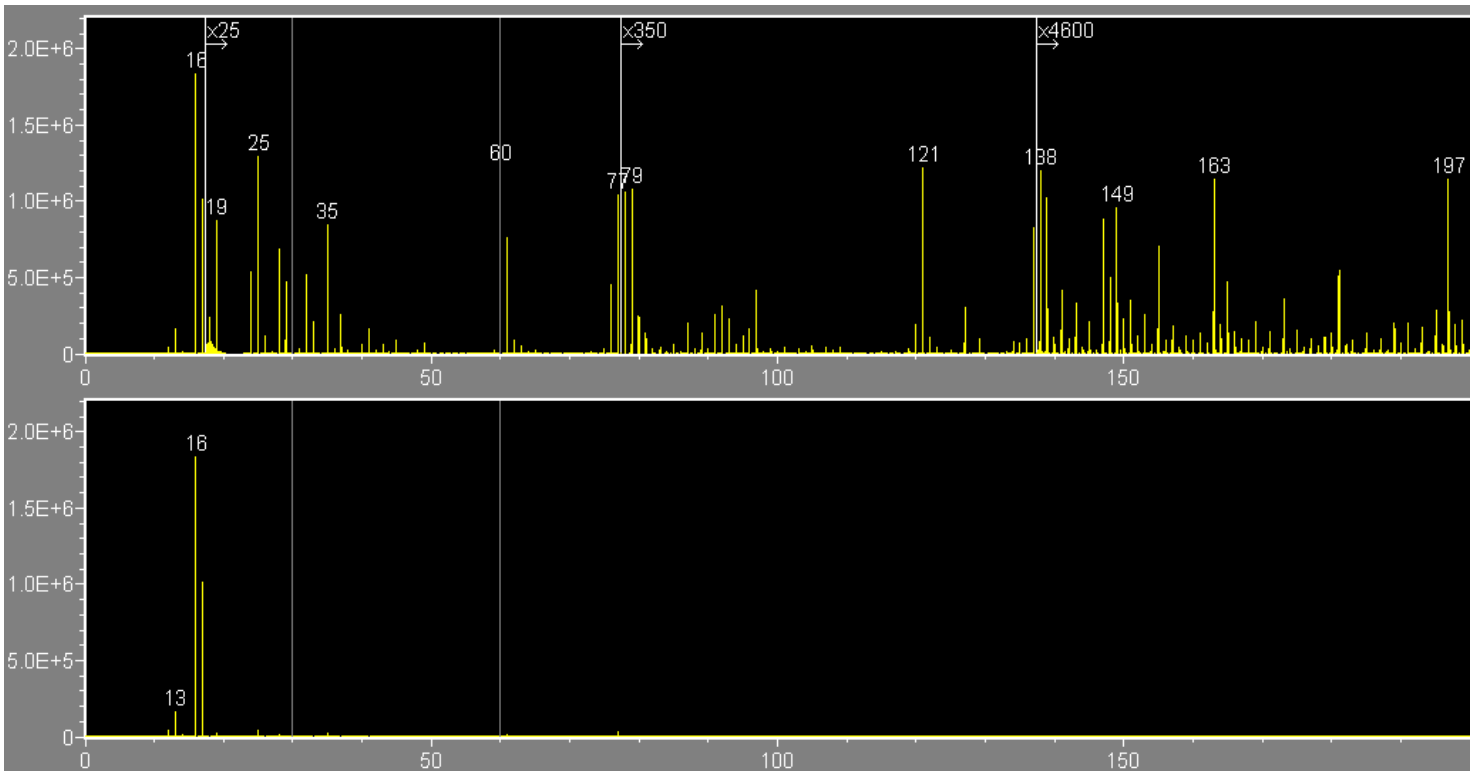


Figure 1 – Spectrum displayed with and without Expanders.

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.

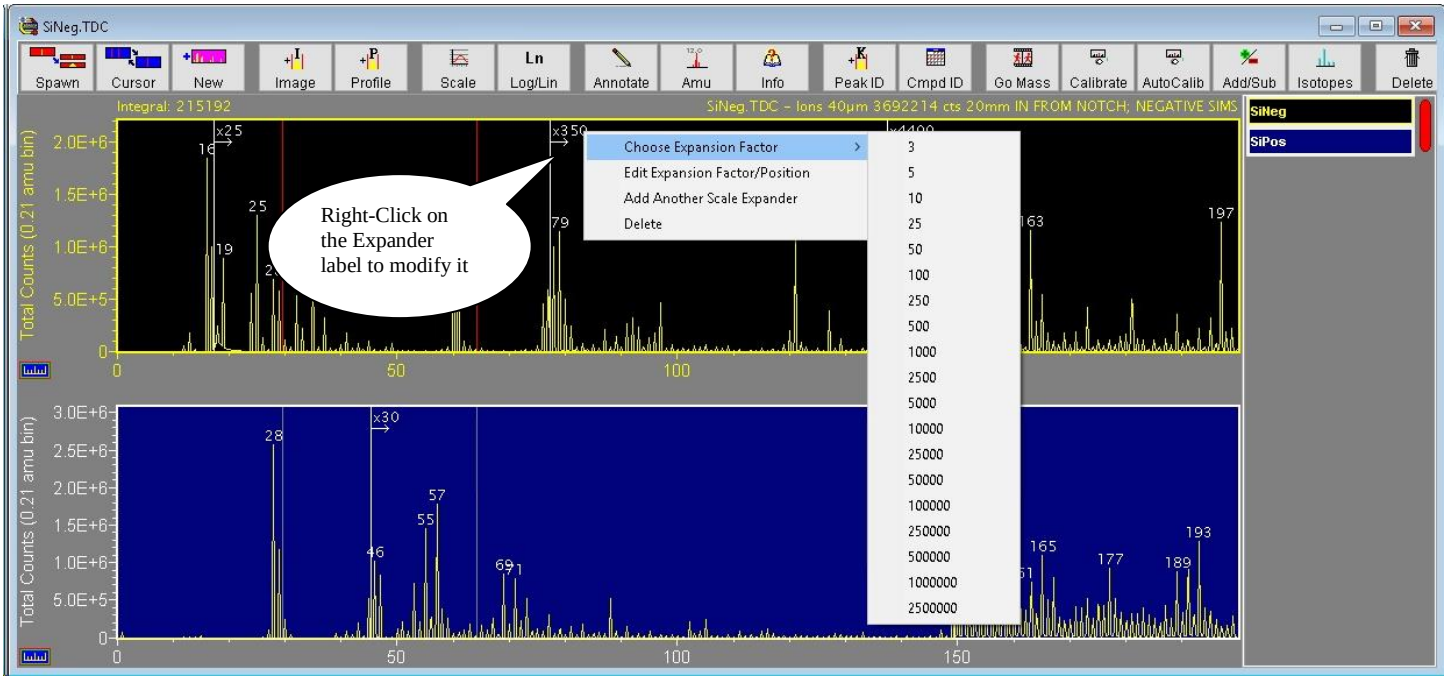


Figure 2 – Right click on the Expander label to modify it

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:

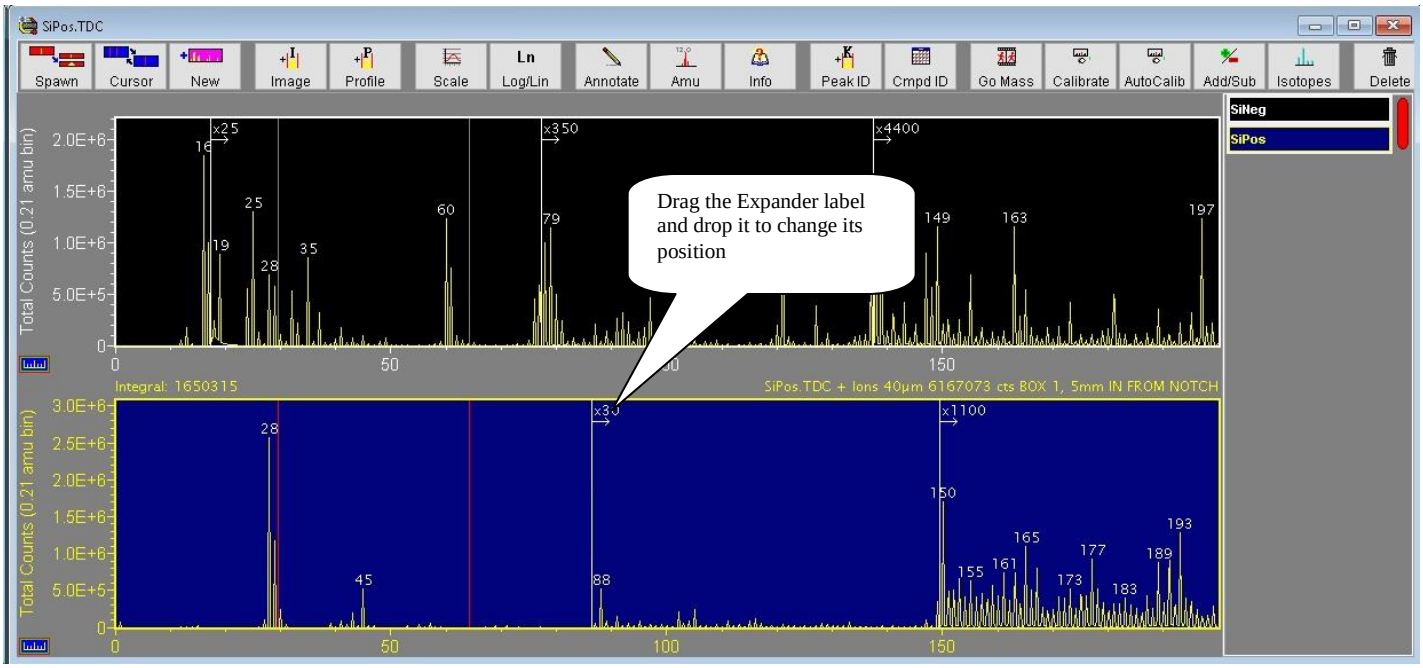


Figure 3 – Drag the Expander label to change its position

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.

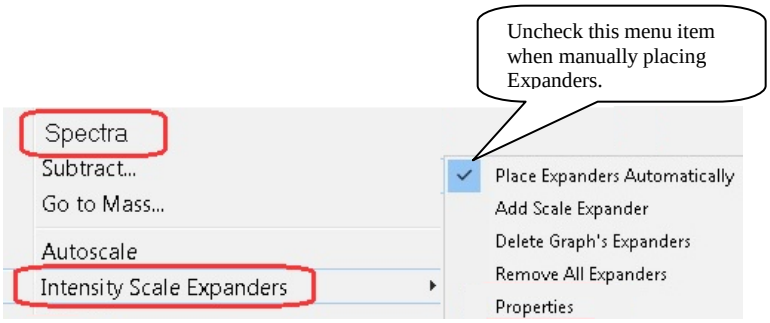


Figure 4 – The Intensity Scale Expanders sub-menu

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.

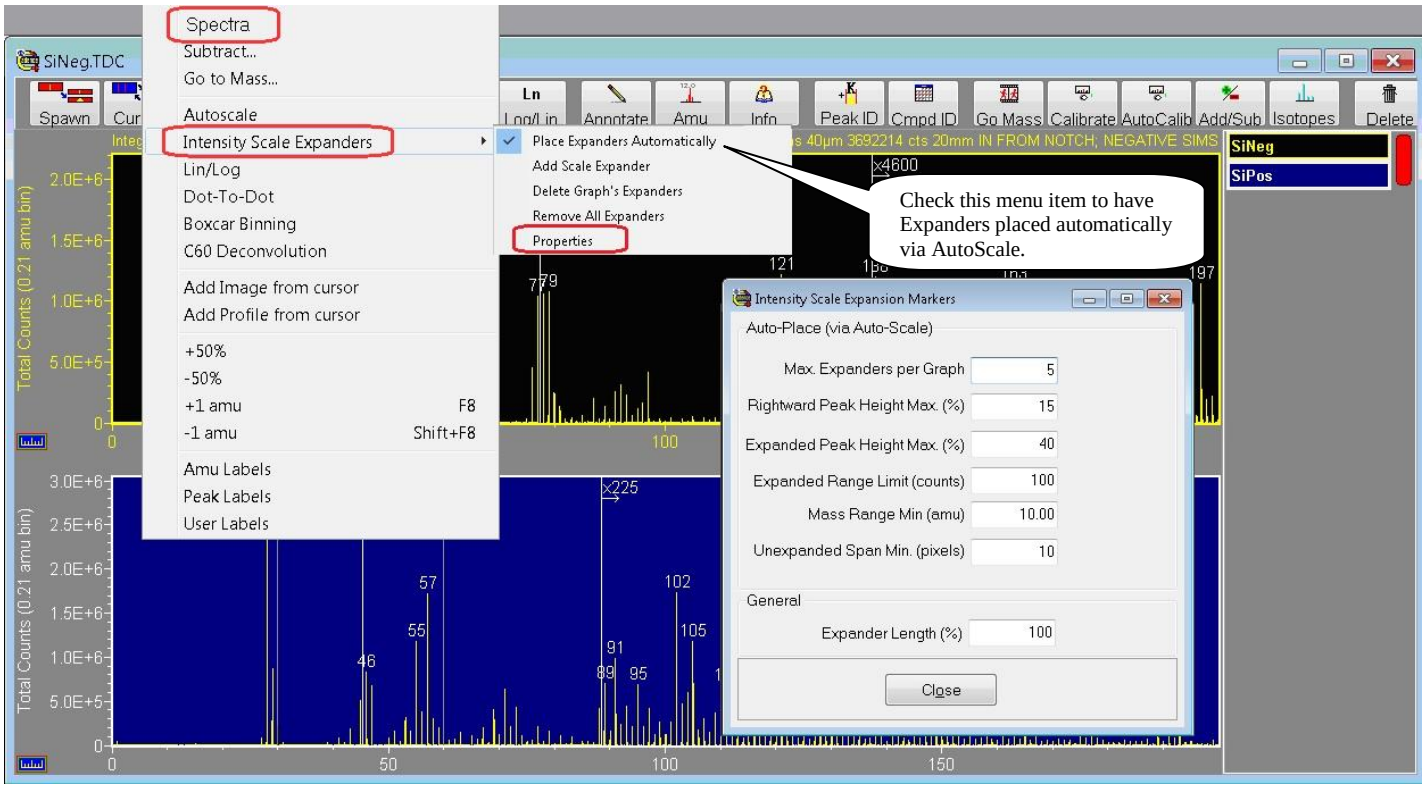


Figure 4 – Properties Dialog for Expanders

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:

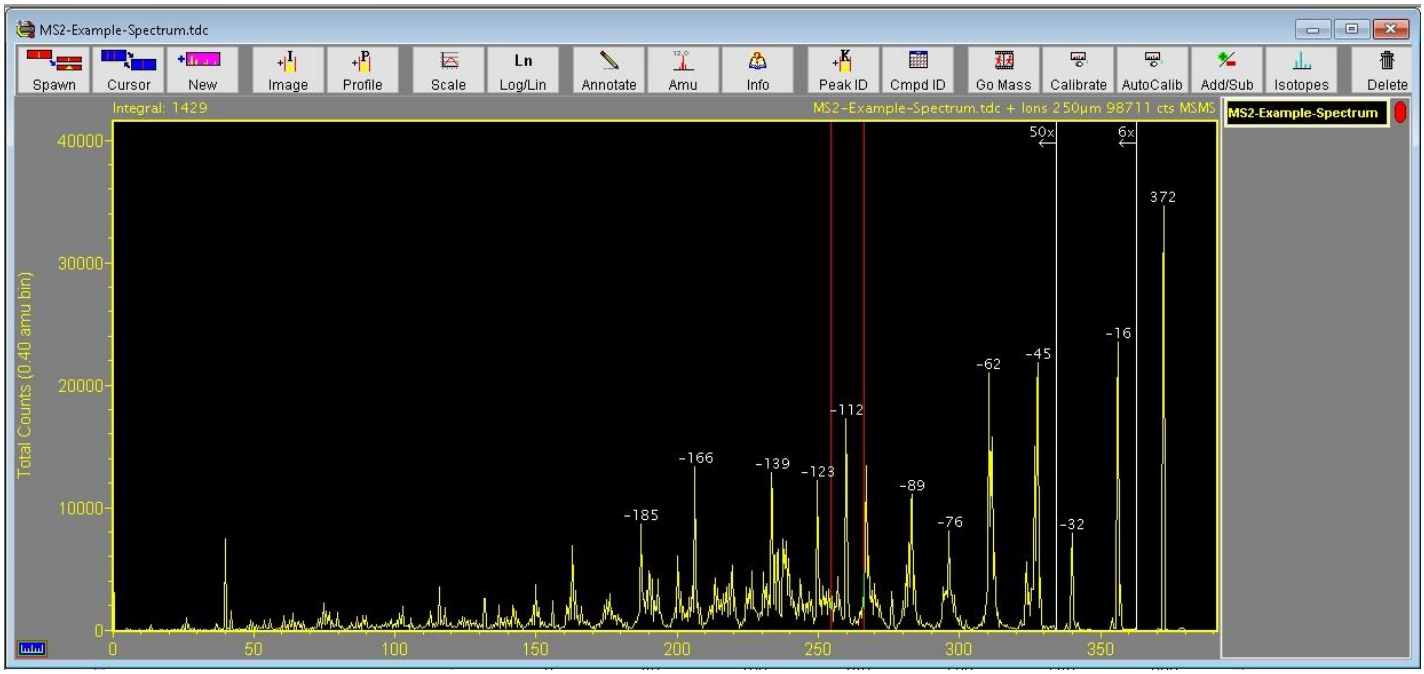


Figure 5 – Expanders operate in the leftward direction for MSMS data

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

TOF-DR Version 1.4

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 $^{28}Si^{+}$, $^{29}Si^{+}$ and $^{30}Si^{+}$ can be grouped together into a single "$\Sigma^{28}Si^{29}Si^{30}Si$" peak-group in the Peak Window as shown below.

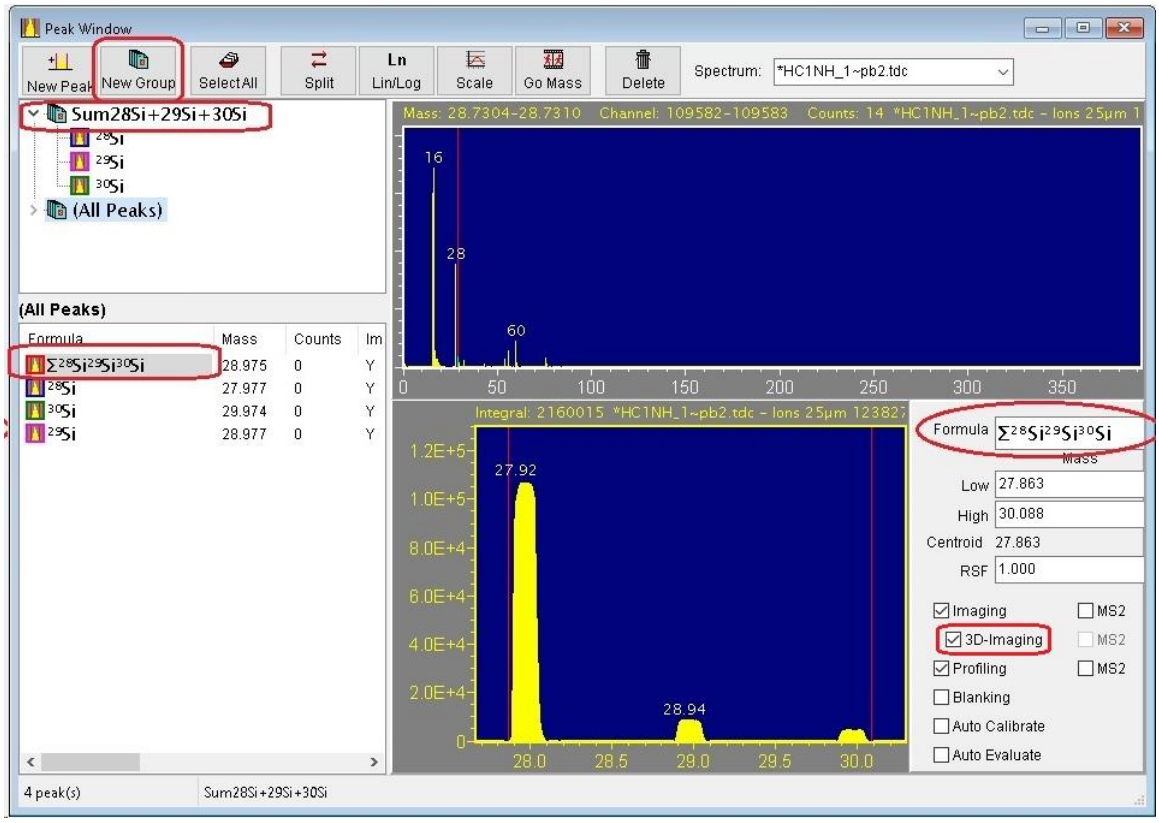


Figure 1 – Peak-Group defined in the Peak Window.

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.

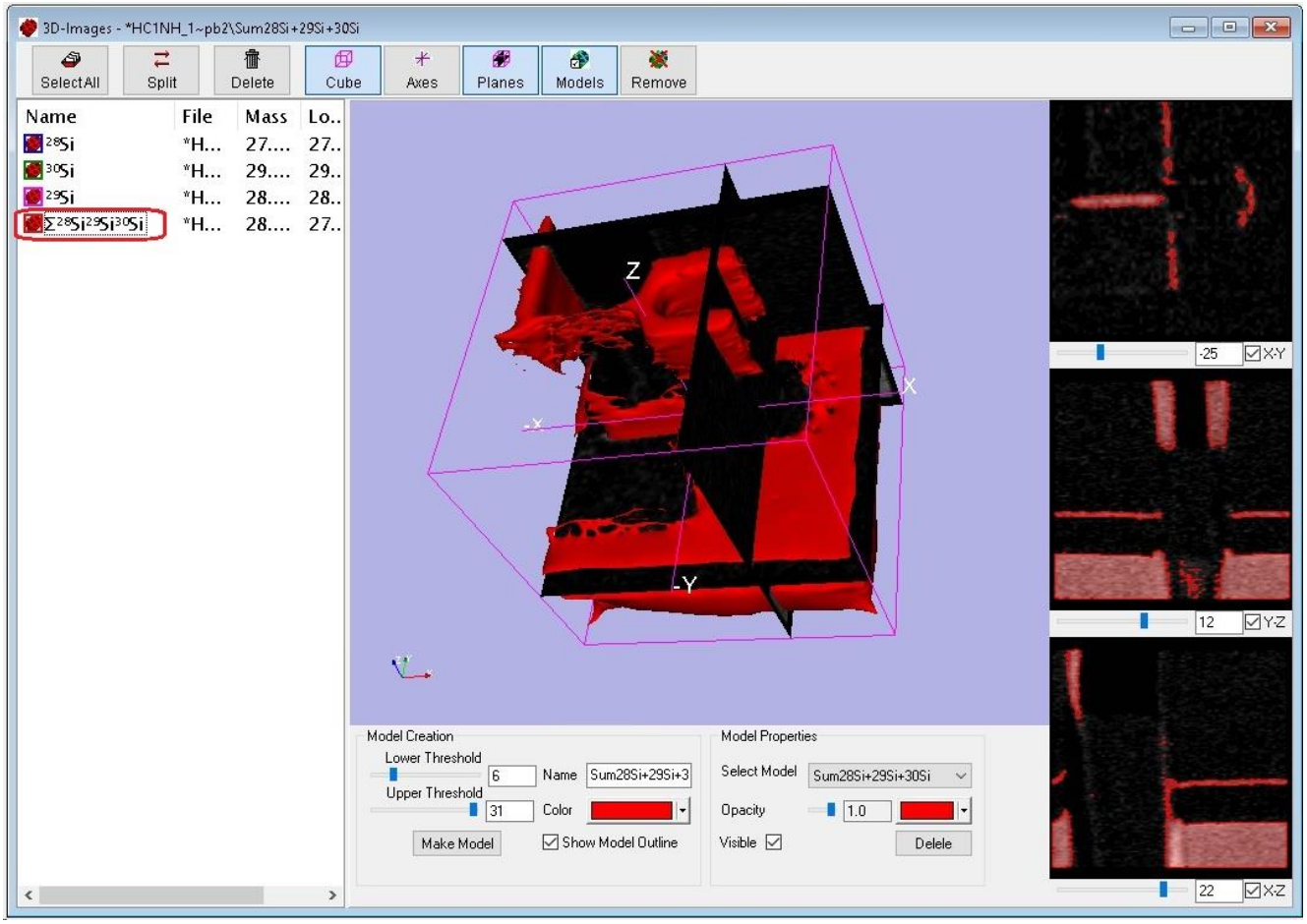


Figure 2 – 3D-Image of a Peak-Group

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.

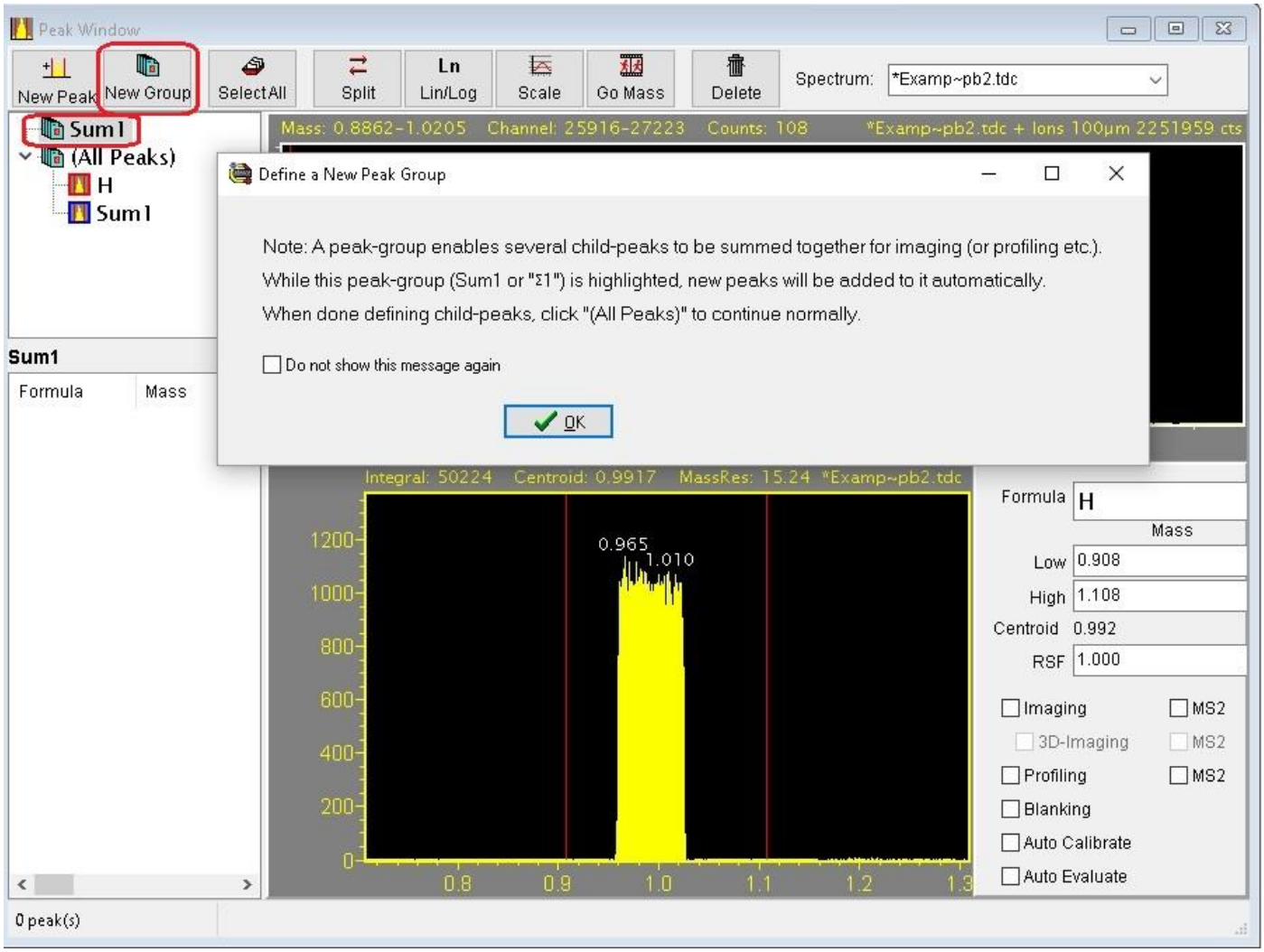


Figure 3 – Defining a New Peak Group

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. “63Cu” as shown below

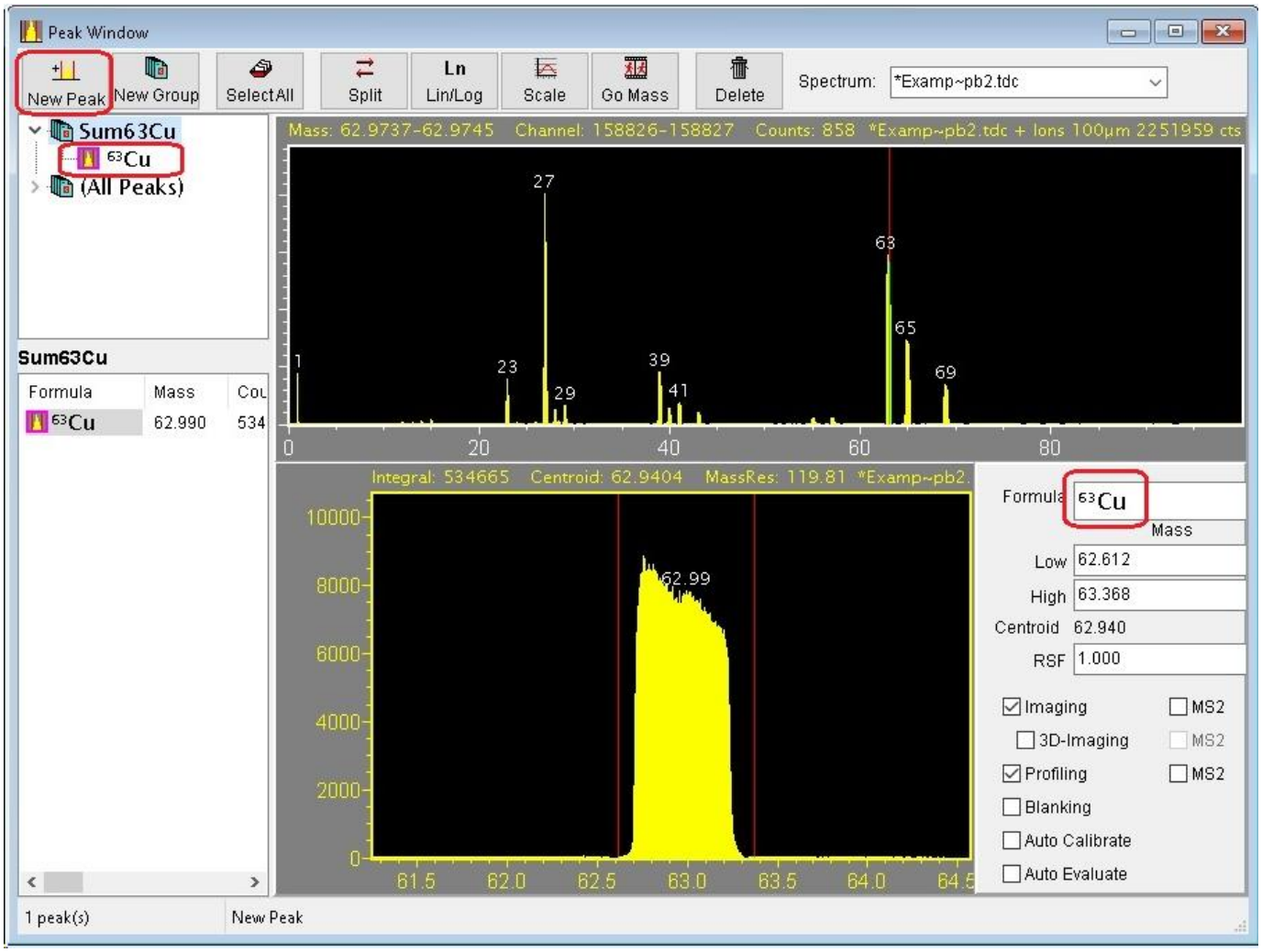


Figure 4 – Defining a 1st Child Peak for a Peak Group

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 “Σ^{63}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. “65Cu” as shown below in Figure 5

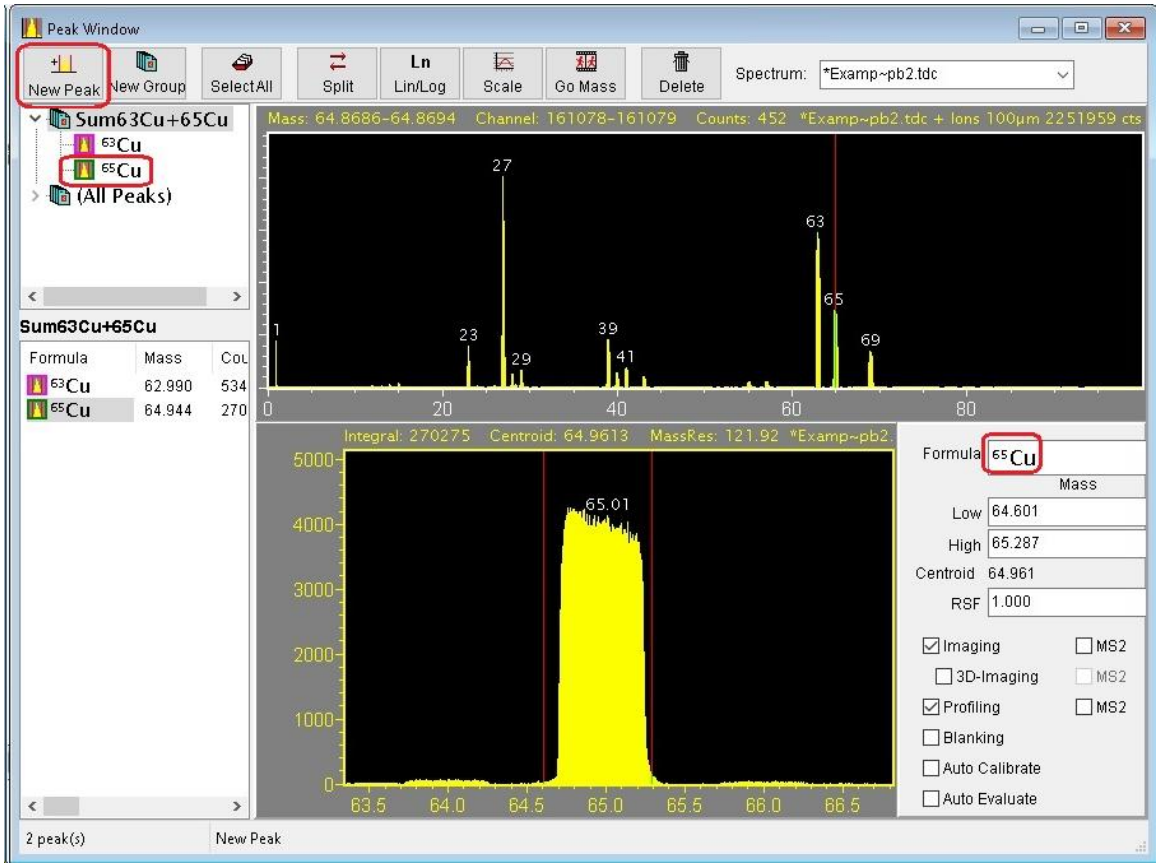


Figure 5 – Defining a 2nd Child Peak for a Peak Group

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 “$\Sigma^{63}Cu^{65}Cu$”) 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.

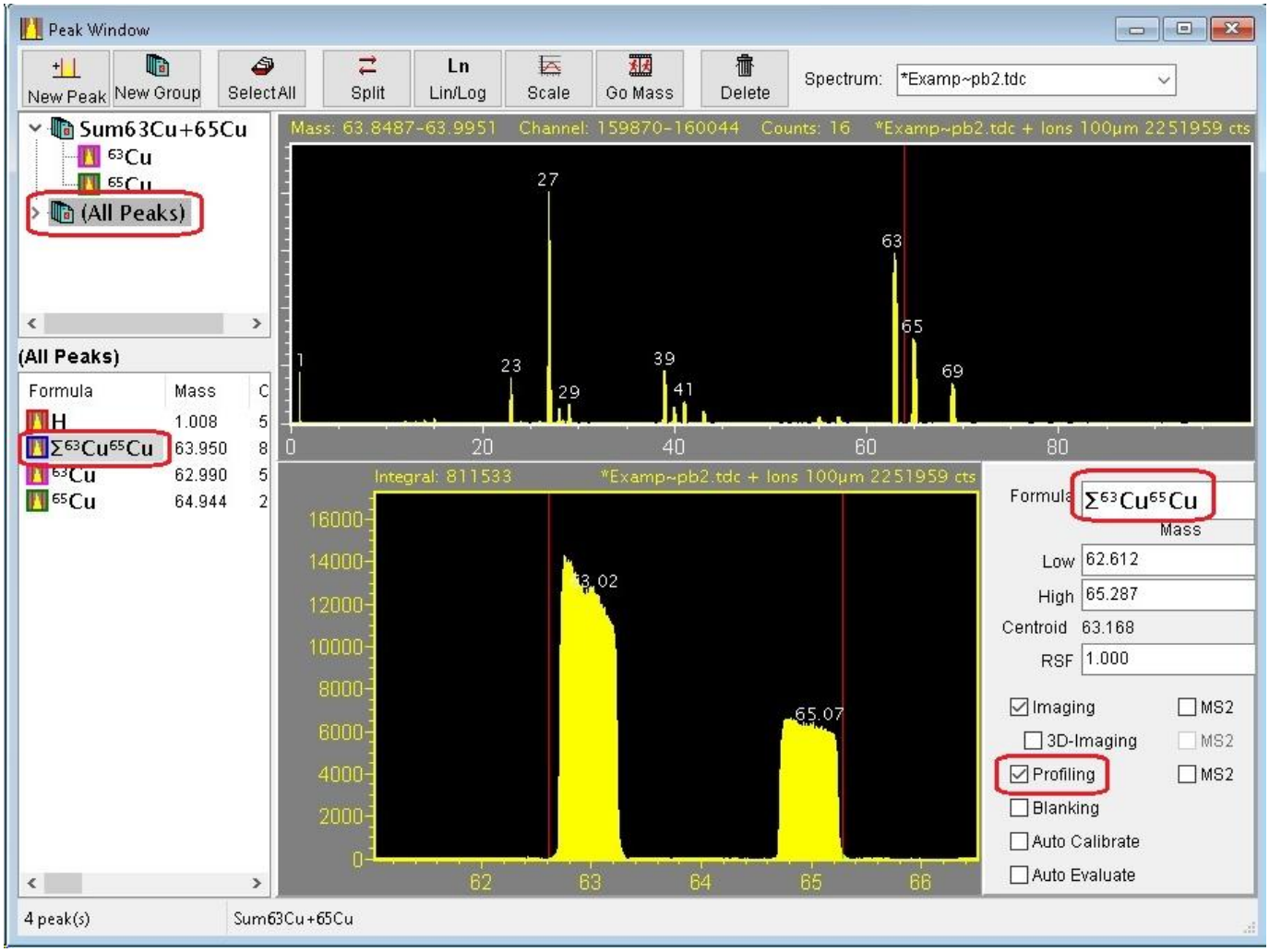


Figure 6 – Setting the Profiling property for a Peak Group

Now click the "$\Sigma^{63}Cu^{65}Cu$" 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.

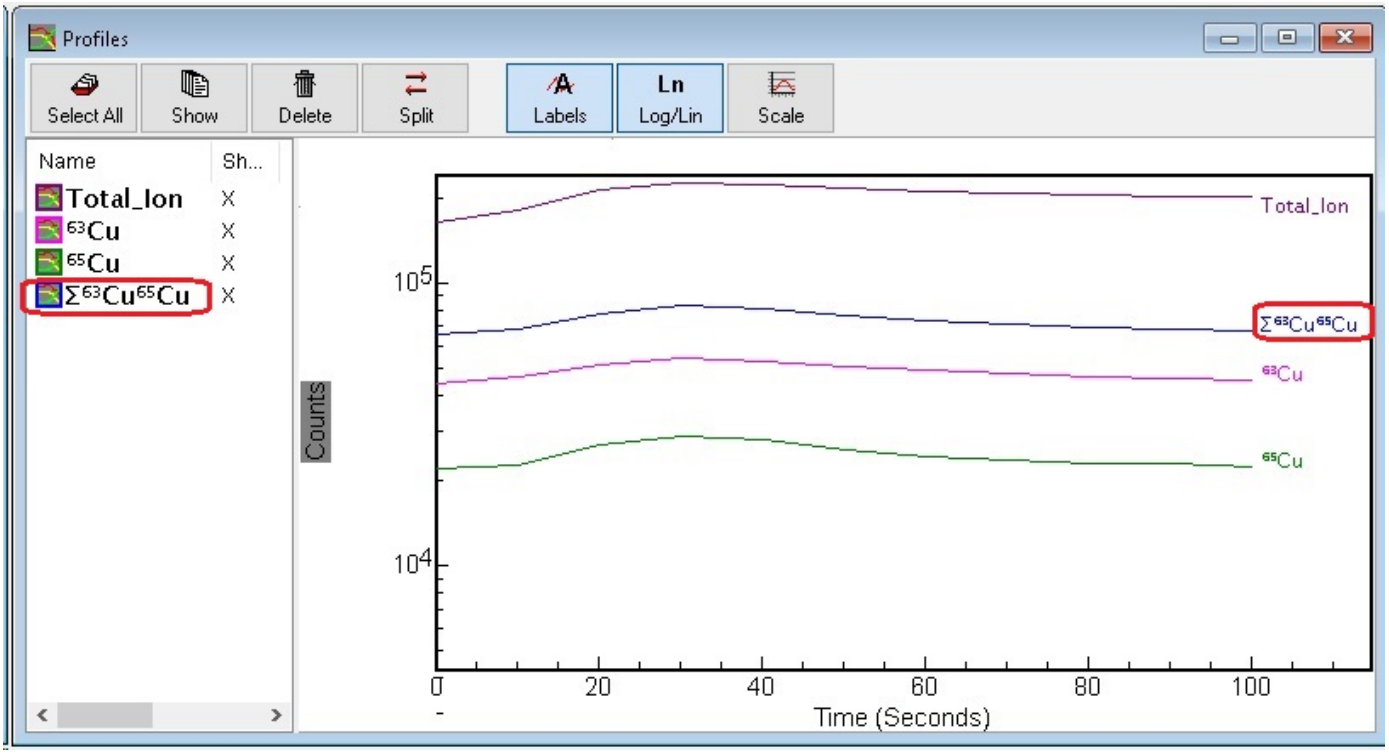


Figure 7 – The Peak Group Profile Curve shown in the Profiles Window

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