

SyncPro Quick Start Manual (Version 1.03)

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1. Introduction

1.1. Brief Description of SyncPro

SyncPro is a java-based visualization package. It compares **multiple processed liquid chromatography-mass spectrometry (LC-MS) or capillary electrophoresis-mass spectrometry (CE-MS) data sets**. The main features of SyncPro are:

1. synchronizing different datasets and different kinds of plots in visualization;
2. facilitating data exploration through selection and extraction;
3. judging the quality of selected features through scatter plots.

You are more than welcome to send your comments and suggestions to us at timyung@ust.hk.

1.2. Installation Guide

You should find the following files and folders under root directory of SyncPro:

Configuration\	-- Folder for configuration files
lib\	-- Folder for library used
ReadMe	-- ReadMe documentation
startSyncPro.bat	-- Executable bat script for Windows
startSyncPro.sh	-- Executable shell script for Linux/Unix
SyncPro.jar	-- Java Executable file

Tested Operating System

- I. Windows XP Professional SP2 (32-bit), Windows XP Professional SP3 (32-bit)
- II. Windows Vista SP2 (64-bit)
- III. Fedora 10
- IV. Novell openSUSE 10.2
- V. Ubuntu 8.04 (32-bit), Ubuntu Intrepid 8.10 (64-bit)

Software Requirements for SyncPro

Operating system : Windows / Linux / Unix

Java Runtime Environment (Version) : 1.6 or above

Default Memory Usage : Minimum - 256 MB, Maximum - 1024 MB

For Windows

You can start SyncPro by running bat file "startSyncPro.bat". If you encounter any problems in starting SyncPro under Windows,

1. Missing of java registry key and no environment variable for java bin directory
Please either provide JAVA_HOME at line 11 in "startSyncPro.bat" or re-install your java to the latest version at <http://java.sun.com/javase/downloads/index.jsp>. (You would probably encounter the problem because you have installed a 32-bit java into a 64-bit windows system without entering java registry key in the correct location.)
2. Java version mismatch or missing of Java executable files.
Please visit <http://java.sun.com/javase/downloads/index.jsp> and update to latest Java Runtime Environment (JRE).
3. Out of memory
Please adjust the memory allocated to SyncPro by changing line 7
"SET JVM_ARGS=-Xms256m -Xmx1024m" in "startSyncPro.bat" (-Xms MINIMUM_MEMORY_ALLOCATED, -Xmx MAXIMUM_MEMORY_ALLOCATED).
A full list of explanations of arguments used by java executable can be found at <http://java.sun.com/javase/6/docs/technotes/tools/windows/java.html>.

For Linux/Unix

You can start SyncPro by running bash shell script "startSyncPro.sh". If you encounter any problems in starting SyncPro under Linux/Unix,

1. Permission denied in execution of SyncPro
Open a bash shell, move to the root directory of SyncPro. Under the root directory of SyncPro, type "chmod a+rx ./startSyncPro.sh", then you can start SyncPro by entering the command "./startSyncPro.sh" in the bash shell.
2. Java version mismatch or missing Java executable files
Please visit <http://java.sun.com/javase/downloads/index.jsp> and update to latest Java Runtime Environment (JRE).
3. Out of memory
Please adjust the memory allocated to SyncPro by changing line 9 "JVM_ARGS="-Xms256m -Xmx1024m"" in "startSyncPro.sh" (-Xms MINIMUM_MEMORY_ALLOCATED, -Xmx MAXIMUM_MEMORY_ALLOCATED).
A full list of explanations of arguments used by java executable can be found at <http://java.sun.com/javase/6/docs/technotes/tools/windows/java.html>.

Special Notes for Linux/Unix

You cannot launch SyncPro using "startSyncPro.sh" bash shell script directly if you wish to access the program on a Linux/Unix server via SSH with X11 (Due to the shift on some internal variables). To access the program on a Linux/Unix server via SSH with X11, you need to use "startSyncPro.sh" to generate the startup script for SyncPro (Just ignore those exceptions when you run "startSyncPro.sh"). SyncPro can be started by copying the startup and execute it directly in a bash shell.

Your bash startup script should be similar to the following example

```
/usr/bin/java
-cp ./SyncPro.jar:./lib/mydoggy-1.4.2/mydoggy-api-1.4.2.jar:./lib/mydoggy-1.4.2/mydoggy-plaf-1.4.2.jar:./lib/mydoggy-1.4.2/mydoggy-res-1.4.2.jar:./lib/mydoggy-1.4.2/TableLayout-20050920.jar:./lib/dom4j-1.6.1/dom4j-1.6.1.jar:./lib/gdswing/gdswing.jar:./lib/jfreechart/jcommon-1.0.16.jar:./lib/jfreechart/jfreechart-1.0.13.jar:./lib/Jrap/jakarta-regexp-1.4.jar:./lib/Jrap/jrap_3.0.jar:./lib/Jrap/jrap-dist.jar:./lib/xerces/resolver.jar:./lib/xerces/xercesImpl.jar:./lib/xerces/xercesSamples.jar:./lib/xerces/xml-apis.jar:./lib/xerces/xmlParserAPIs.jar:./lib/apache-log4j-1.2.15/log4j-1.2.15.jar:./lib/apache-commons-math-2.0/commons-math-2.0.jar -Xms256m -Xmx1024m Main
```

1.3. Acknowledgement of various resources

A number of open source software packages are used in SyncPro. These packages and corresponding links are listed as follows:

Core software packages:

- Program logging – Log4j and Xerces from the Apache Software Foundation
<http://www.apache.org>
- MZXML file parsing – JRAP mzXML parser in the Trans-Proteomic Pipeline software developed by the Seattle Proteome Center
<http://tools.proteomecenter.org/wiki/index.php?title=Software:JRAP>
- XML file parsing – Dom4j in the apache Maven Project
<http://www.dom4j.org/index.html>
- Chart drawing – JFreeChart from JFree.org
<http://www.jfree.org/>
- Graphical user interface docking framework – MydoggyFramework
<http://mydoggy.sourceforge.net/>
- Internal desktop management – Swing Desktop extensions by Guy Davis
<http://www.guydavis.ca/log/view.jsp?id=893>
- Statistical Score Calculation –The Apache Commons Mathematics Library
<http://commons.apache.org/math/>

Miscellaneous source codes and resources:

- Relative path generator – A java class written by David M. Howard
<http://www.devx.com/tips/Tip/13737>
- Magnifier len and memory monitor – Java classes written by Angelo De Caro and included in the package of MyDoggyFramework
- Silk icon set – A set of icons provided by Mark James
<http://www.famfamfam.com/lab/icons/silk/>

2. Components of SyncPro

2.1. Inputs and outputs of SyncPro

2.1.1. Inputs

mzML

mzML¹ is a new mass spectrometry data format proposed by Deutsch from Institute for Systems Biology, Seattle, WA, USA. Some well-known software packages like Trans-Proteomic Pipeline (TPP) and X!Tandem have accepted it as a standard input format. SyncPro supports inputting mzML (version 1.1.0) files and all visualization plots are available for this format. The specification of mzML is available at <http://www.psidev.info/index.php?q=node/257>.

mzXML

mzXML is one of the most widely used proteomics data formats. SyncPro accepts preprocessed mzXML files and adds them as file nodes in the project tree. Current version of SyncPro uses a simple rendering scheme to render **all data points** in file nodes. It is not recommended to input unprocessed mzXML files into SyncPro. Users may suffer from poor rendering performance, especially for the 2D-intensity plot. For details of the format of mzXML, please visit <http://tools.proteomecenter.org/wiki/index.php?title=Formats:mzXML>.

TSV feature file of MSInspect

TSV file is a feature file generated from feature detection algorithms of MSInspect (Bellew et al., 2006)². SyncPro visualizes detected features from MSInspect as plots for further comparisons. Please refer to <http://proteomics.fhcrc.org/CPL/msinspect/index.html> for working principles of feature detection algorithms and the format of tsv file.

¹ Deutsch E. mzML: a single, unifying data format for mass spectrometer output. *Proteomics* 2008, 14:2776-2777.

² Bellew, M., Coram, M. Fitzgibborn, M., Igra, M., Randolph, T., Wang, P., May, D., Eng, J., R., and Lin, C. W. (2006). A suite of algorithms for the comprehensive analysis of complex protein mixtures using high-resolution LC-MS. *Bioinformatics*, 22(15), 1902-1909.

Rawfile

Rawfile is an input format introduced in SyncPro. It is a simple file format with the structure shown in Fig. 1. The file is composed of blocks of data. Each block represents a single scan and is separated by a blank line. The first line of a scan is the scan number and retention time. The remaining lines are peaks in the scan. Each line starts with the m/z value and continues with the intensity value of the corresponding peak.

```
D:\CEMS Peak Result\Convert\061222D000003.D_bruker.rawfile - Notepad++
File Edit Search View Format Language Settings Macro Run TextFX Plugins Window ?
061222D000003.D_bruker.rawfile
1 14 PT42.614000s
2 622.4155 24.0
3 650.52386 25.0
4 700.4571 23.0
5 1088.3887 16.0
6 1604.2697 23.0
7
8 15 PT45.635000s
9 590.3554 42.0
10 610.16583 34.0
11 611.3145 29.0
12 650.4589 28.0
13 717.4436 19.0
14 1274.2554 16.0
15 1740.2577 19.0
16
17 16 PT48.656000s
18 599.331 31.0
19 610.16583 43.0
20 611.346 25.0
21 634.4501 25.0
22 638.70715 24.0
23 641.38104 26.0
24 642.3973 33.0
25 650.5401 25.0
26 659.4534 30.0
27 666.6179 27.0
28 675.359 37.0
29 701.6709 23.0
30 1067.6305 21.0
31
32 17 PT51.679000s
33 606.3971 23.0
34 610.16583 48.0
35 616.726 40.0
36 624.4027 29.0
37 630.78284 47.0
38 632.36694 39.0
39 633.4882 24.0
40 636.4882 36.0
41 650.5401 31.0
42 654.476 17.0
43 660.66394 25.0
Normal text file nb char : 11800808 Ln : 9 Col : 14 Sel : 0 UNIX ANSI INS
```

Fig. 1 An example of raw file

2.1.2. Outputs

Featurefile

Featurefile is a self-defined exporting format in SyncPro. It includes information of threshold values for feature points in the feature tool window tab (see Fig. 2). The first line contains threshold values and number of features in that feature file. The threshold values include retention time threshold and m/z threshold used by the tab to search for existed feature points in different datasets. For the remaining lines in the featurefile, each line represents a feature point. It starts with retention time value and continues with m/z value of that feature point.

```
C:\Documents and Settings\Timyung\Desktop\MSVis Runnable\Project\FatureGermanyDataProject\RawFile\Project1\FatureGermanyDataProject1_FeatureFile.featurefile - Notepad++
File Edit Search View Format Language Settings Macro Run TextFX Plugins Window 2
GermanyDataProject1_FeatureFile.featurefile
1 100.000000, 0.100000, 10
2 2299.199951, 1725.589966
3 1866.000000, 1834.819946
4 1738.800049, 2742.250000
5 1512.000000, 4321.939941
6 1750.199951, 1451.660034
7 1729.199951, 1378.609985
8 2389.800049, 1491.739990
9 1202.400024, 5276.410156
10 2263.800049, 1624.550049
11 2086.199951, 2471.149902
12
Normal text file nb char : 263 Ln : 7 Col : 24 Sel : 0 UNIX ANSI INS
```

Fig. 2 An example of feature file

2.2. Overview of SyncPro

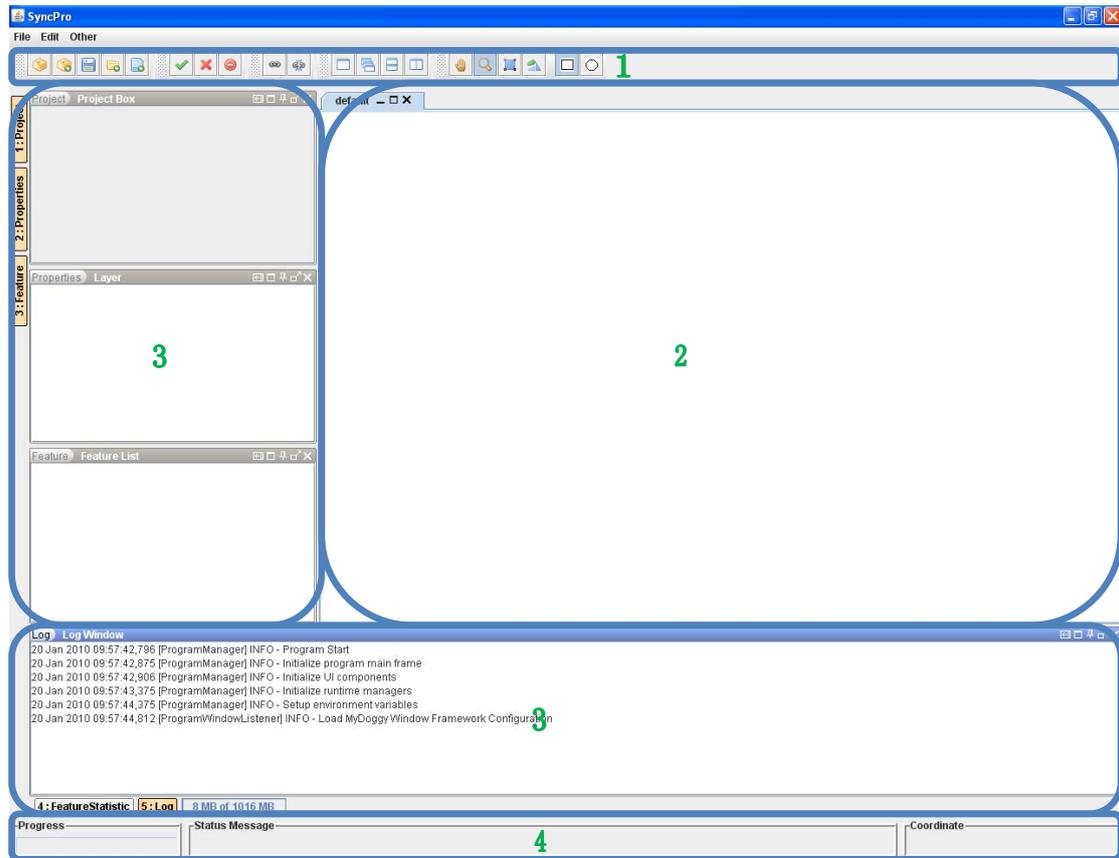


Fig. 3 Overview of SyncPro

1. Program tool bar (Details in section 2.2.1)
Program tool bar provides quick access points to frequently used functions.
2. Program desktop pane (Details in section 2.2.2)
Program desktop pane displays various plots. File nodes from the project panel can be dragged and dropped to the pane and visualized as different plots.
3. Program tool window tabs (Details in section 2.2.3)
Program tool window tabs have various functions. The project tab manages the files in the project. The layer properties tab shows layer information for spectrum plots. The feature tab holds feature points and statistical information of files in the project. The log tab records program log messages.
4. Program status bar (Details in section 2.2.4)
Program status bar shows some hotspot messages such as the coordinate information in a specific plot and the latest program operation.

2.2.1. Program tool bar



Fig. 4 A closer view of program tool bar

Project management functions

1. Create a new project by specifying a working directory and a project name.
2. Open an existed project.
3. Save the current project.
4. Create a folder under a selected project node or folder node.
5. Add files from a dialog to the selected folder node in the project tree.

Visibility functions for the file nodes in the project tree

6. Make nodes visible.
7. Make nodes invisible.
8. Remove nodes.

Linkage functions for the program desktop pane

9. Link all internal frames in the selected desktop pane.
10. Remove links among all internal frames in the selected desktop pane.

Tile functions for internal frames in the program desktop pane

11. Tile frame proportionally.
12. Tile frame cascadelly.
13. Tile frame vertically.
14. Tile frame horizontally.

Working modes for the 2D-intensity plot

15. Set the 2D-intensity plot working in the pan mode
16. Set the 2D-intensity plot working in the zoom mode.
17. Set the 2D-intensity plot working in the selection mode.
18. Set the 2D-intensity plot working in the rotation mode.

Selection shape for selection mode of the 2D-intensity plot

19. Set the selection shape to be a rectangle.
20. Set the selection shape to be an ellipse.

2.2.2. Program desktop pane

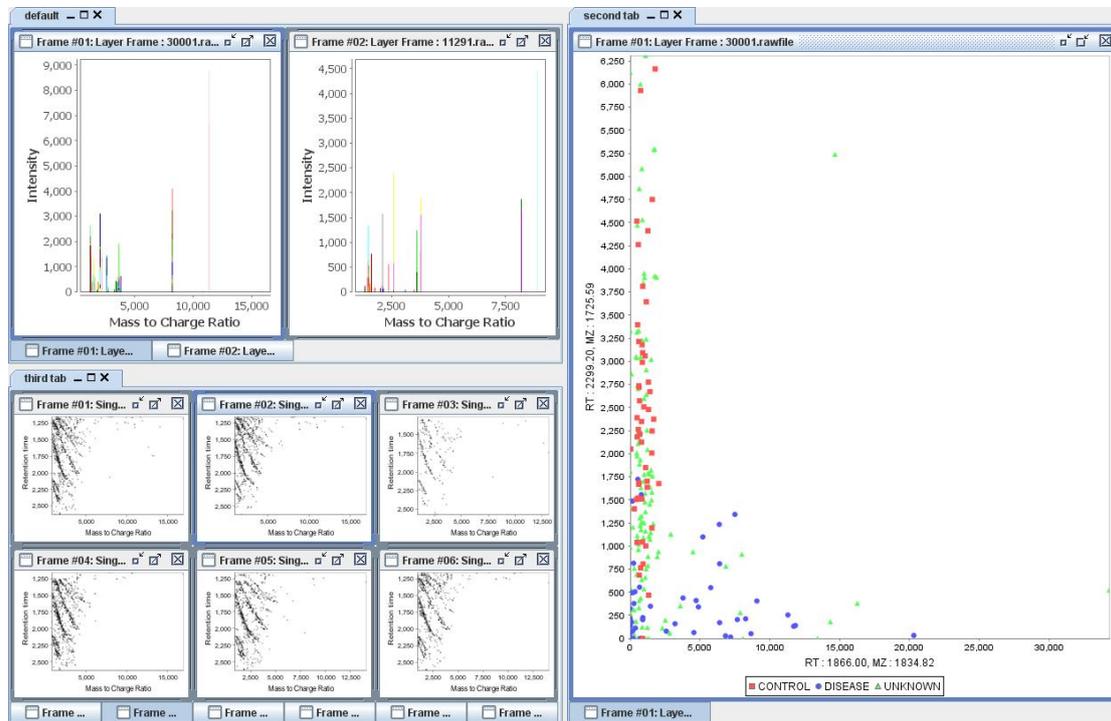


Fig. 5 A demo for having various plots in the program desktop pane

- File nodes can be dragged and dropped to any tab in the program desktop pane and visualized in desired plots.
- Each tab in the program desktop pane can be linked individually using linkage buttons in the program tool bar.
- Tile operations can be performed via tile options in the program tool bar.

Remarks:

For a specific tab in the desktop pane, users can click on any internal frame in that tab to set the focus on that tab. All link and tile operations will then apply to the tab in focus.

2.2.3. Program tool window tabs

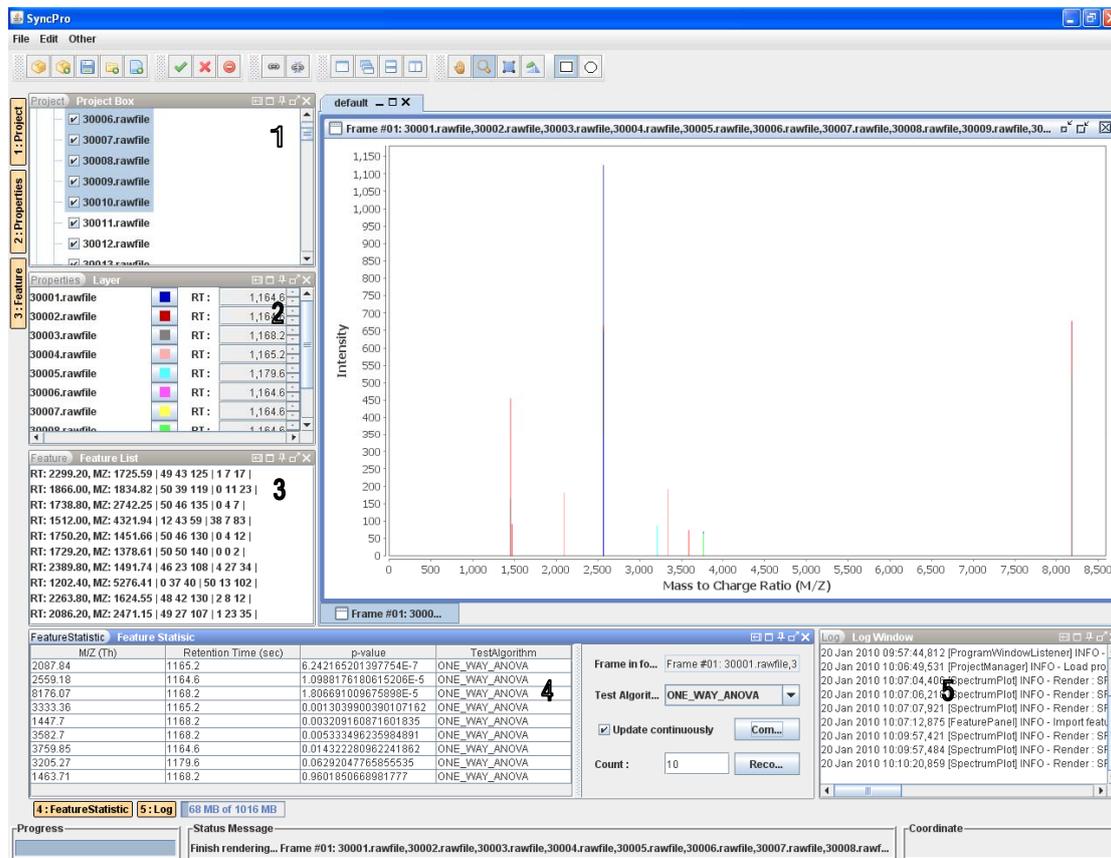


Fig. 6 Screenshot for different tool window tabs in SyncPro

- 1. Project tool window tab**
 The tab displays a project as a tree, users may manipulate the project by simply dragging and dropping tree nodes, using the buttons in tool bar, or using the popup menu by right clicking on selected nodes.
- 2. Layer tool window tab**
 Information for different layers in the spectrum plot is shown in the tab. The peaks of a scan from a dataset are represented as a series of color bars in the spectrum plot. The color of a scan can be changed by clicking on the color icon. Scans from the same file can be examined by varying the spinner.
- 3. Feature tool window tab**
 Potential features are added in the tab from spectrum plots or directly entered via options provided in the popup menu of the tab. Users can have some statistical information of feature points in different file nodes of the current project.

4. Feature statistic tool window tab
Data points of the frame currently in focus are treated as feature points and statistic scores are computed using various algorithms based on the information of files in entire project. The scores are displayed as records in the table of this tab.
5. Log tool window tab
Program log messages are recorded in this tab for tracking project manipulation and logging errors.

Remarks:

To enable multiple tool windows, users may hold the “Shift” key and click on the tab labels on the boundary of SyncPro program.

2.2.4. Program status bar

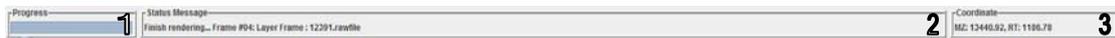


Fig. 7 A closer view of program status bar

1. Progress Tab
This tab shows the progress of the latest task (most likely a rendering task).
2. Status Message Tab
This tab shows the status message of the latest task.
3. Coordinate Tab
This tab shows coordinate information of the plot.

3. Tutorial

In this section, the notation {#index} is used to describe marked options in a specified graph (usually a graph of tool bar options).

3.1. Project Management

There are three types of nodes in the project tree. They are project node, folder node and file node. A project node starts with a package icon ; a folder node starts with a folder icon ; and a file node starts without any icons. The project is organized as a tree and users can manipulate the project with the help of options in Fig. 8.



Fig. 8 Tool bar options for project management

3.1.1. Managing nodes in the project

Creating a folder in the project tree

1. Select the project node or a folder node in the project tree.
2. Click on {4} (see Fig. 8), a dialog is shown and requests for the folder name (see Fig. 9).
3. Enter the folder name and click on the "OK" button to finish the process.

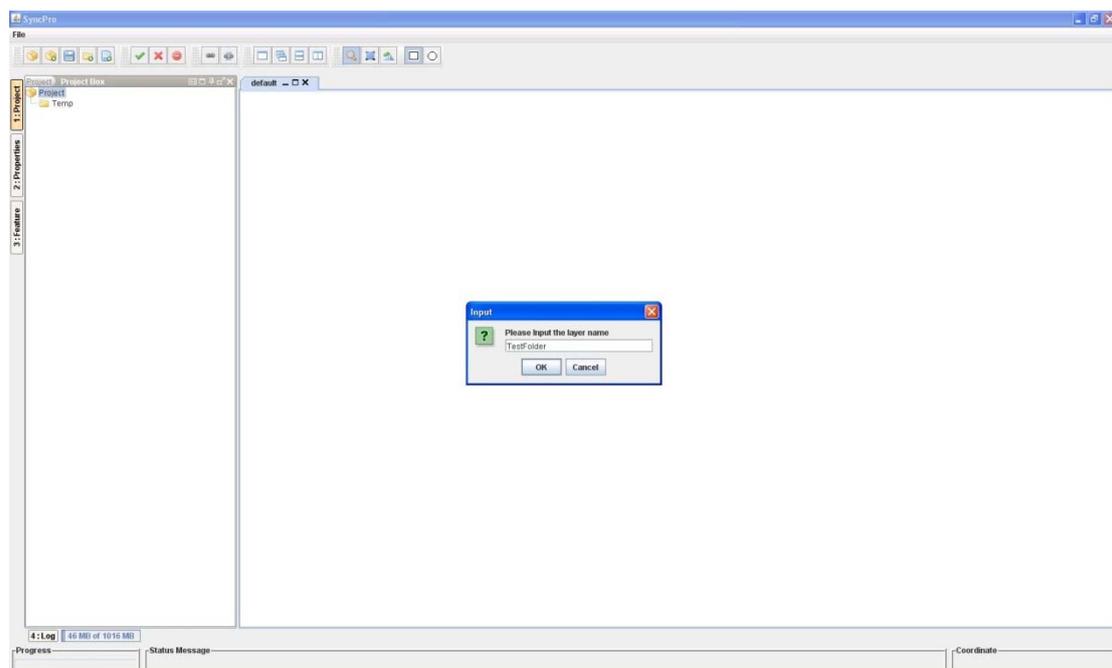


Fig. 9 Creating a folder "TestFolder" under the project node

Adding files to the project tree

1. Select a folder node in the project tree.
2. Perform a click on {5} (see Fig. 8). A file open dialog shows up and requests for files (see Fig. 10).
3. Select multiple files to be added by holding “Shift” or “Ctrl” key.
4. Finish the adding process by clicking on the “Open” button in the file open dialog.

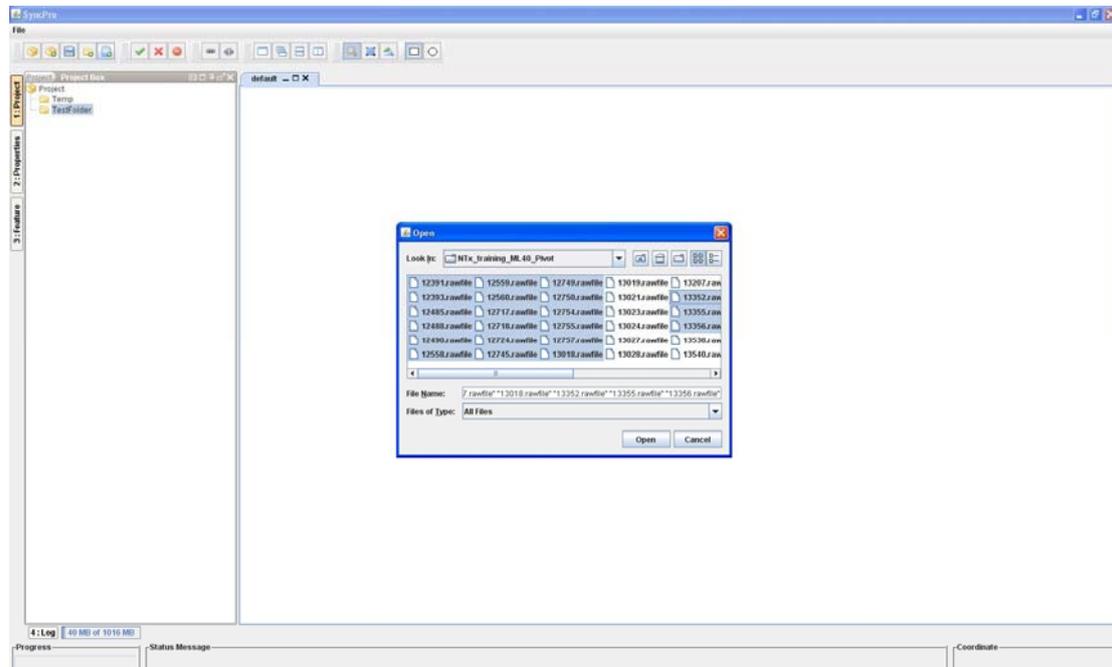


Fig. 10 Adding multiple rawfiles to "TestFolder"

Removing files from the project tree

1. Select multiple folder nodes or file nodes in the project tree by holding “Shift” or “Ctrl” key.
2. Perform a click on {6} (see Fig. 8). All the selected nodes in the project tree will be deleted.

Moving file nodes / Copying file nodes

1. Select multiple file nodes in the project tree by holding “Shift” or “Ctrl” key.
2. Drag and drop the file nodes to the desired position in the project tree.
Copy the file nodes by holding “Ctrl” key, then drag and drop the file nodes to the desired position in the project tree (see Fig. 11).

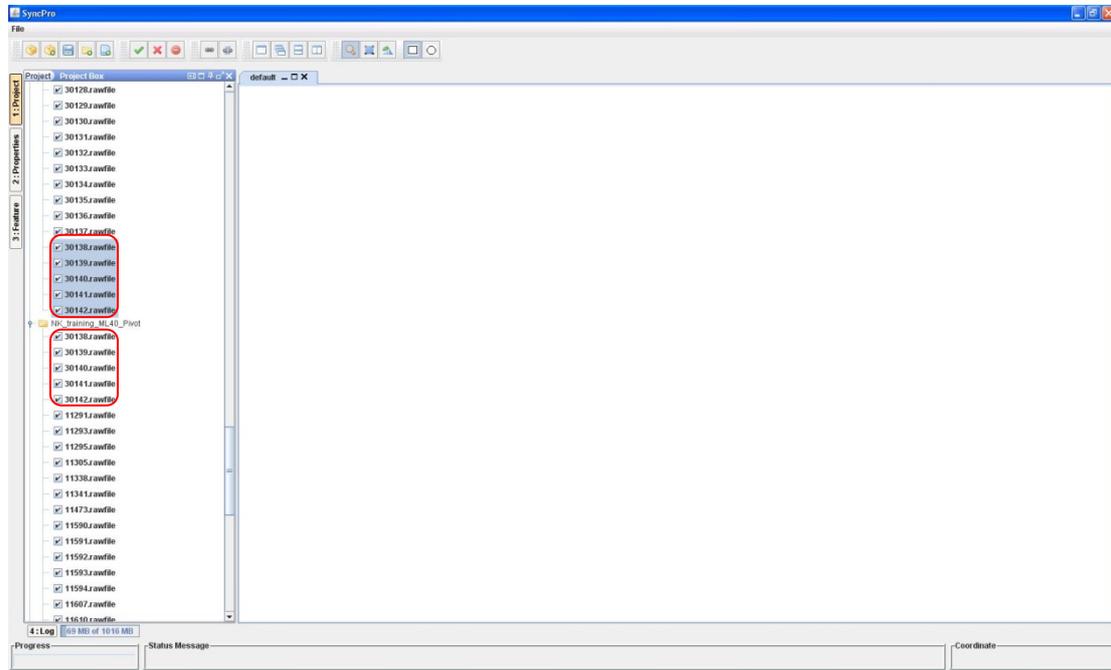


Fig. 11 Copying last five nodes from a folder to another folder

3.2. Visualizing file nodes and related plot functions

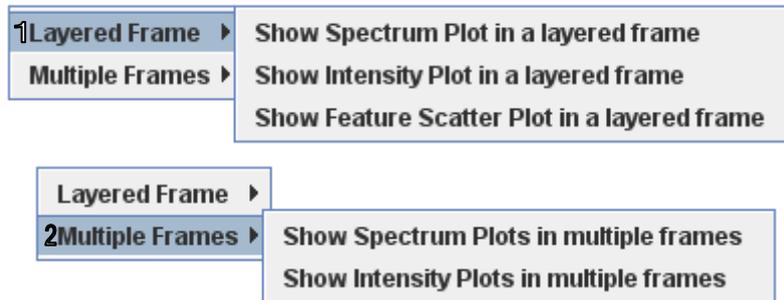


Fig. 12 Drop menus for the files from the project tree

1. Layered frame – Selected file nodes will be added to the same internal frame and rendered as layer in the frame. The rendering order follows the order of file nodes in the project tree.
2. Multiple frames – An individual internal frame will be created for each selected file node. The frame will only visualize the contents of the selected file node.

Visualizing file nodes

1. Select multiple folder nodes or file nodes in the project tree by holding “Shift” or “Ctrl” key.
2. Drag and drop the nodes to the desired tab in the program desktop pane, a drop menu will appear (see Fig. 12).
3. Select the favorite type of plots and add desired plots as internal frames in the tab of the program desktop pane.

Remarks:

Only selection of same type of nodes can trigger drop actions. No drop menu will show up if users select file nodes and folder nodes at the same time and intent to drop them to a tab in the program desktop pane.

3.2.1. 2D-intensity plot

2D-intensity plot shows the distribution of data points among different proteomics data files. A data point with lower intensity will be a darker point in the 2D-intensity plot.



Fig. 13 Tool bar options for 2D intensity plot

Extracting the contents using a rectangular/ellipsoid window

1. Zoom in a 2D intensity plot to a desired scale.
2. Change the working mode of 2D intensity plot to “Selection Mode” ({2} in Fig. 13).
3. Select the desired selection type (rectangle / ellipse, {4} and {5} in Fig. 13).
4. Move the mouse to the top left corner of the selection.
5. Hold and drag the mouse until a desired selection size is reached (see Fig. 14).

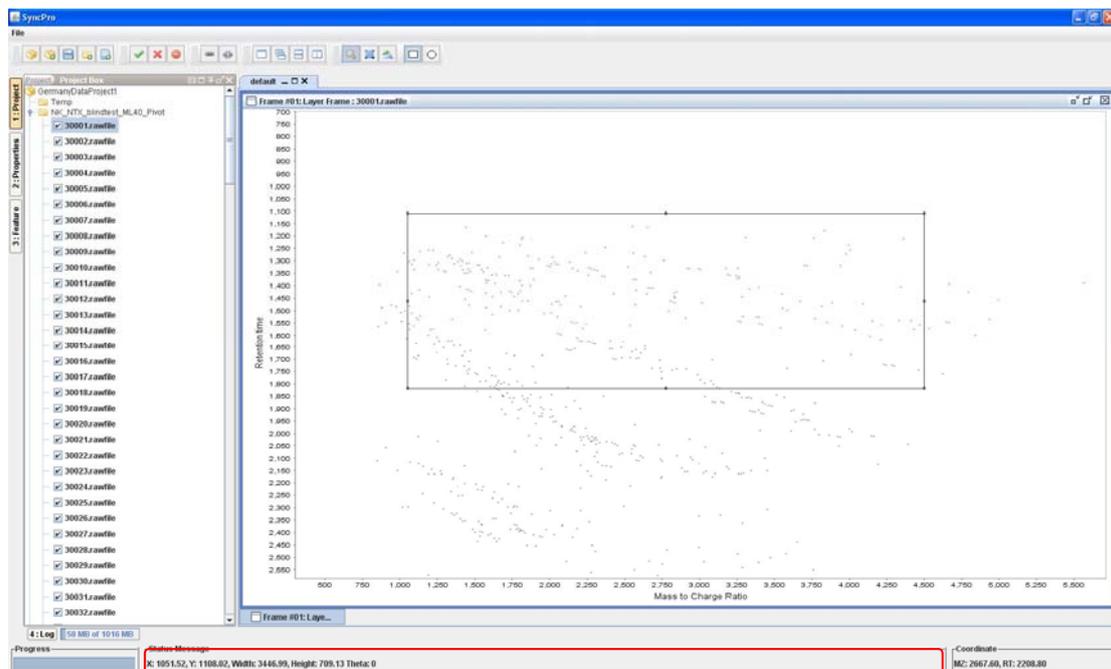


Fig. 14 Making a selection in a 2D-intensity plot

6. Check the selection information in the message tab of the program status bar.
7. Adjust the size at the boundary edge of the selection if necessary.
8. Change the working mode of 2D intensity plot to "Rotation Mode" (3) in Fig. 13).
9. Click and hold the mouse's left button on any points within the selection.
10. Drag the mouse until desired rotation angle is achieved (see Fig. 15).

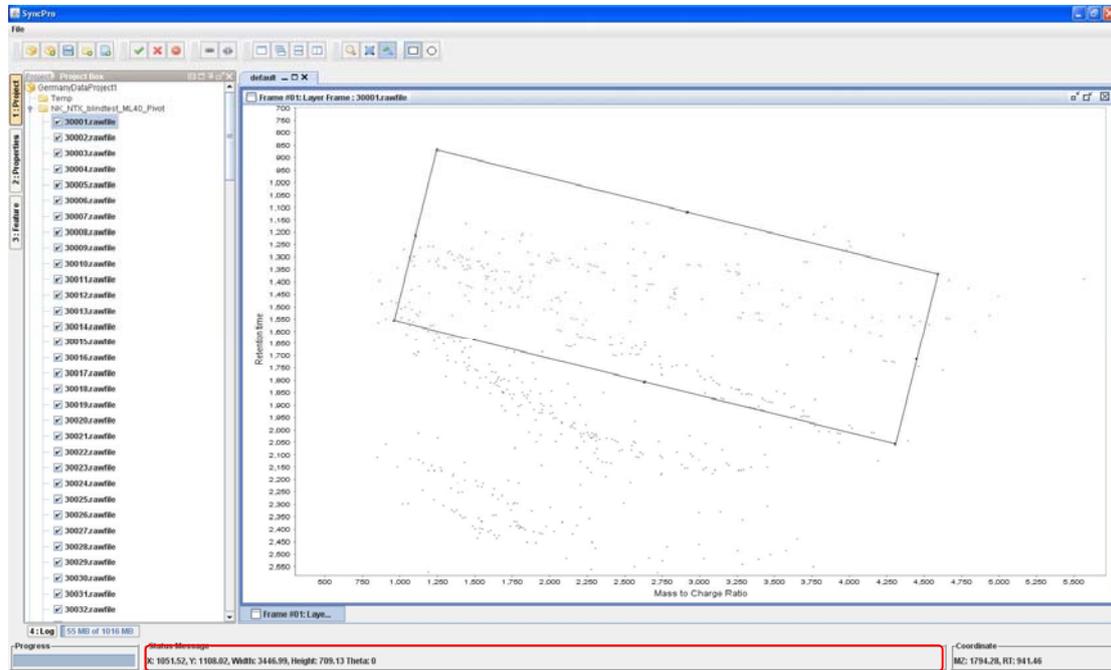


Fig. 15 A rotated window in the 2D-intensity plot

11. Return to “Zooming Mode” (1) in Fig. 13) or “Selection Mode” (2) in Fig. 13).
12. Choose the option “Extract Selection Data”. The selected contents will be extracted and a temp file node will be added to the “Temp” folder in the project tree (see Fig. 16).

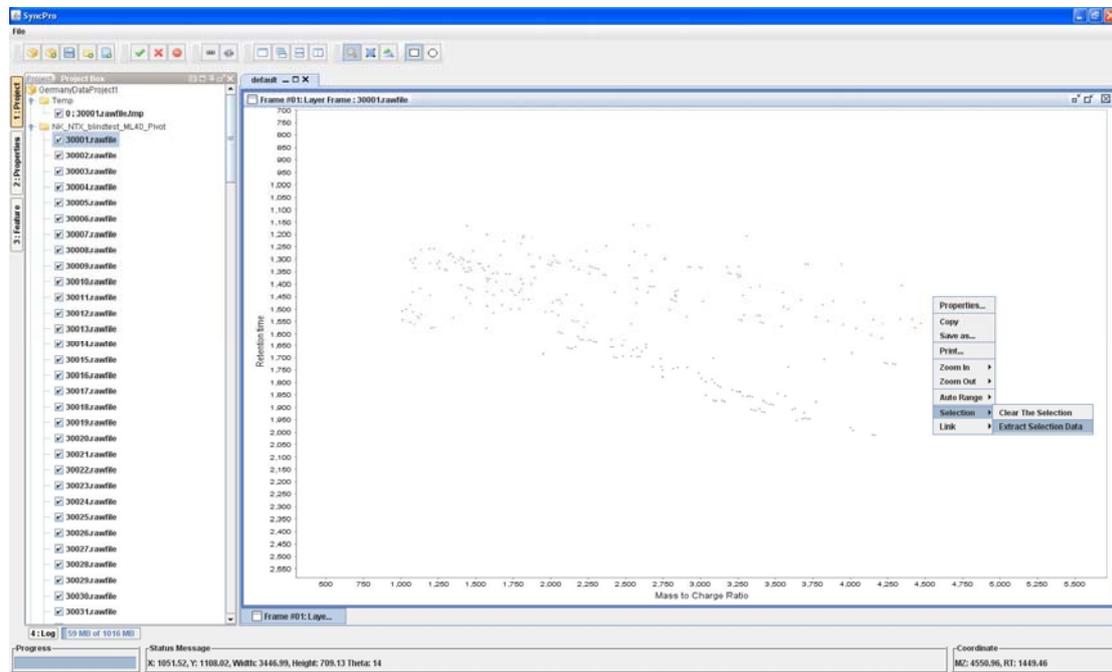


Fig. 16 An extracted area in the 2D-intensity plot

Remarks:

Users can erase the old selection and create a new selection by holding “Ctrl” key during the process of dragging for selection area.

3.2.2. Spectrum plot

Unlike a 2D-intensity plot showing overviews of file nodes, a spectrum plot requires input of retention time in order to show a spectrum. SyncPro will then automatically find the spectrum with the closest retention time to the user input in each file node and add spectra from all nodes into a spectrum plot with layers or spectrum plots.

Changing scans shown in the current spectrum plot

1. Enable the “Layer Property” tool window tab by clicking on the tab label “Properties” in the left boundary of SyncPro program.
2. Gain the focus of a spectrum plot by clicking any area within the plot, the layer information of the spectrum plot will be shown in the “Layer Property” tool window tab (see Fig. 17)

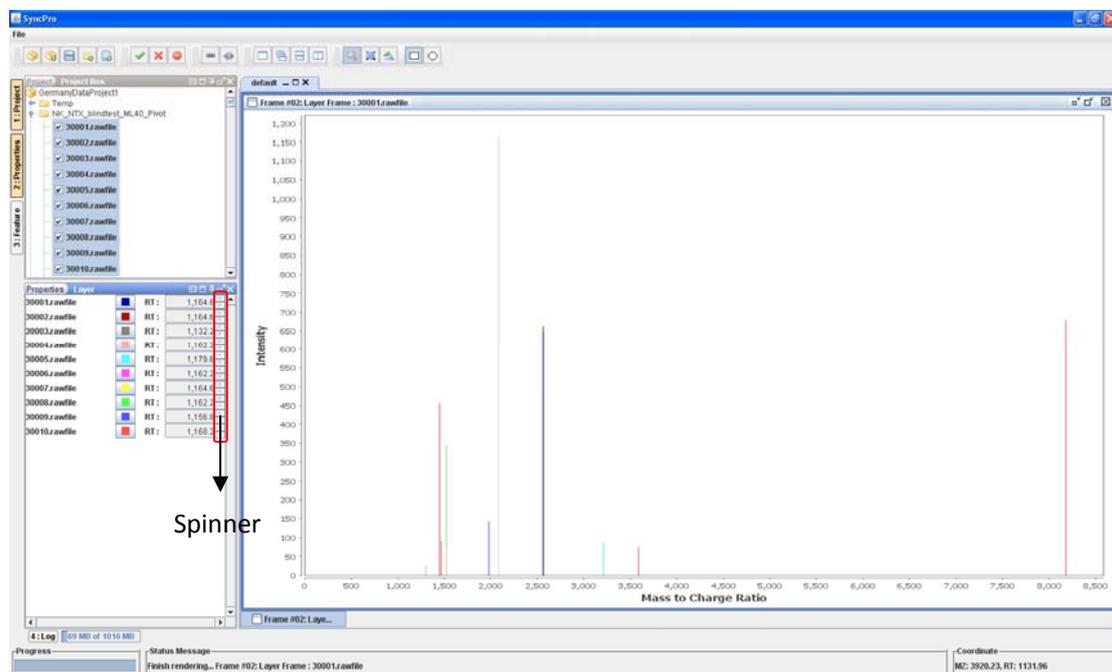


Fig. 17 Spinner for browsing scans from the same file

3. Vary the spinner to examine scans from the same file.

Modifying the color of scan in the spectrum plot

1. Enable the “Layer Property” tool window tab by clicking on the tab label “Properties” in the left boundary of SyncPro program.
2. Click on any area within the spectrum plot to gain the focus, the layer information of the spectrum plot will be shown in the “Layer Property” tool window tab (see Fig. 18)
3. Click the color icon of a file. A color chooser will be prompted (see Fig. 18).
4. Select desired colors to distinguish different scans in the spectrum plot.

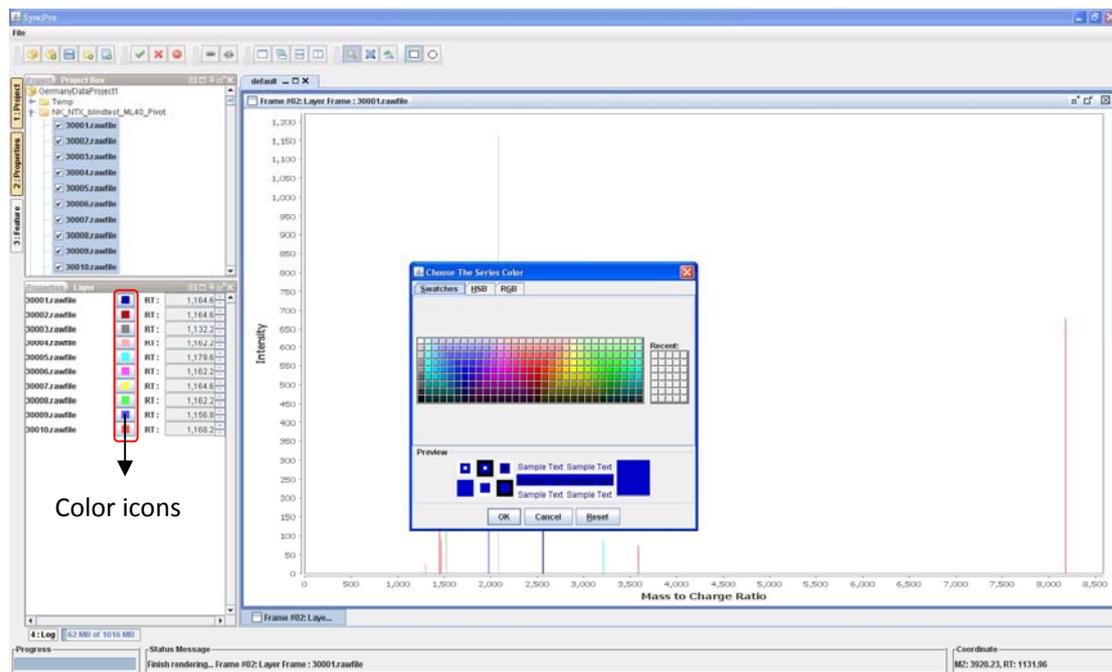


Fig. 18 A color chooser for choosing color of a spectrum

Judging the potential of a data point to be a useful feature point in a spectrum plot

1. Identify an interested scan and open it as a spectrum plot.
2. Choose a suitable test algorithm for current data sets, p-value of all data points are computed based on information of all data files in current project. Their results are displayed as a table (sorted in ascending order by p-value) (see Fig. 19).
3. Choose other test algorithms if a comparison of p-value from different algorithms is desired.
4. Check the p-value in the sorted table, those data points with extremely low p-value would be potential feature point to be further investigated in a feature scatter plot.

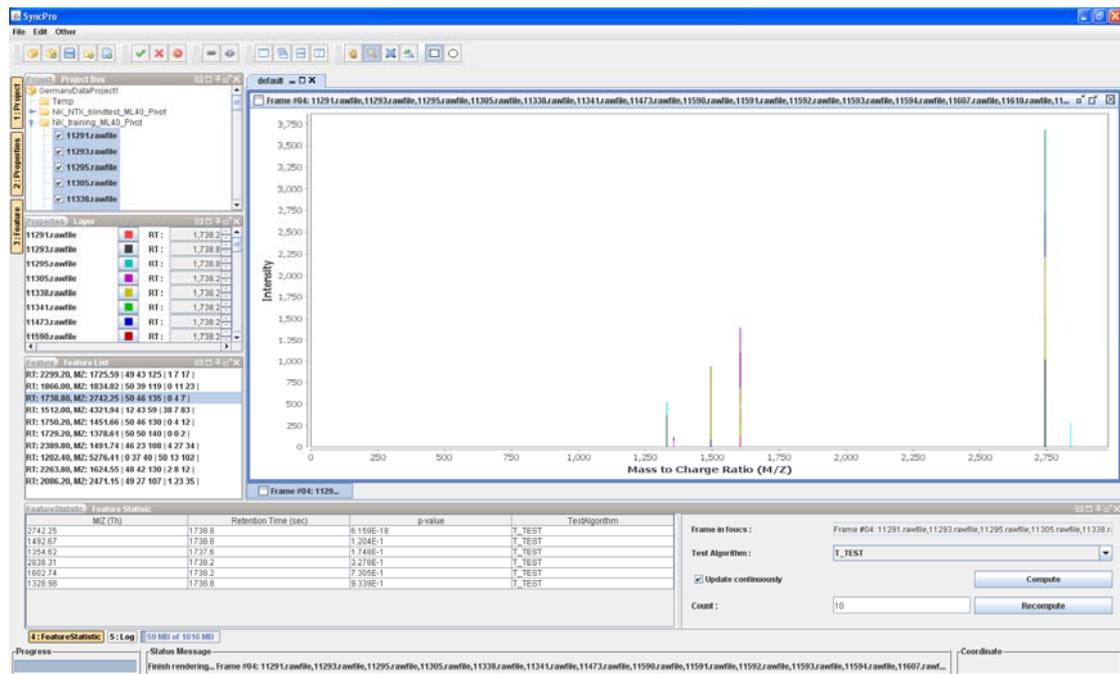


Fig. 19 Presenting p-values of feature points of a spectrum plot

Selecting a data point to be a feature

1. Zoom in the spectrum plot to a desired scale.
2. Change the color of the spectrum if necessary.
3. Right click on any bar (which represents a data point in the file node) of the spectrum plot. The selected information will be displayed in the message tab of the program status bar (see Fig. 20).
4. Verify the data point and add if the feature tool window tab using the option "Select as a feature" in the popup menu.
5. Check the existence of selected feature in the list of the feature tool window tab (see Fig. 20).

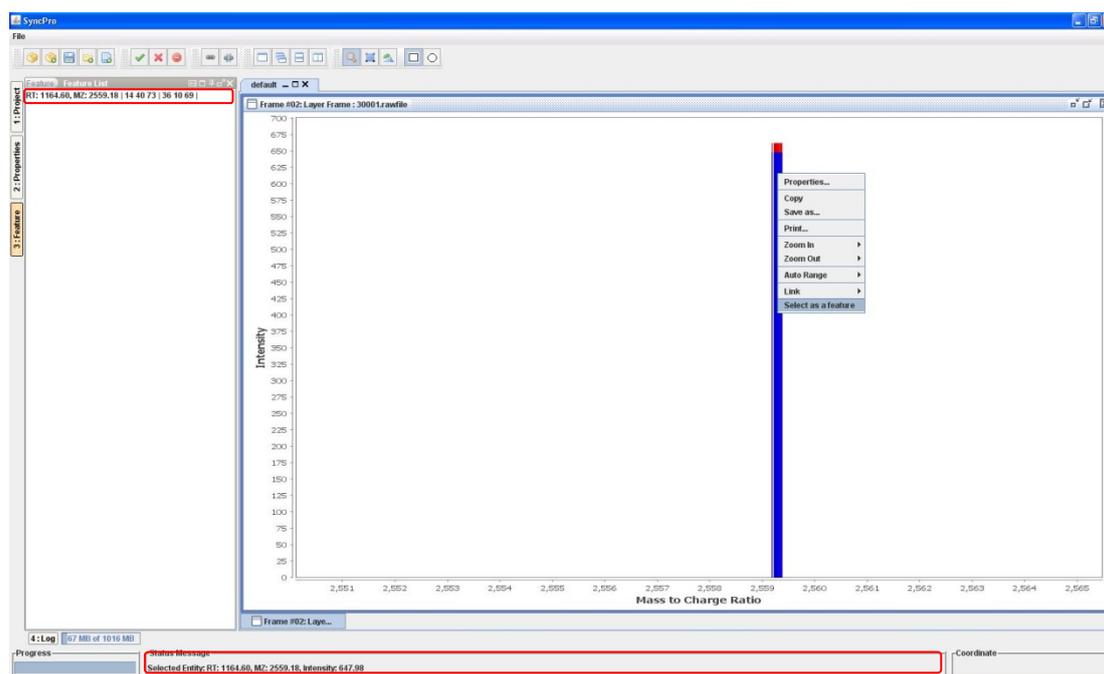


Fig. 20 Adding feature point to the feature tool window tab

Remarks:

A good feature is a point showing strong contrast between the disease group and the control group. One way to discover potential feature points is to overlay multiple file nodes in the spectrum plot. Potential feature points are those data points with large number of different color bars within a short range (typically within an m/z difference of 0.1 Da).

3.2.3. Feature scatter plot

To verify whether selected feature points are good criteria to classify file nodes into different groups, users can select a number of file nodes from the project tree and visualize them in a feature scatter plot.

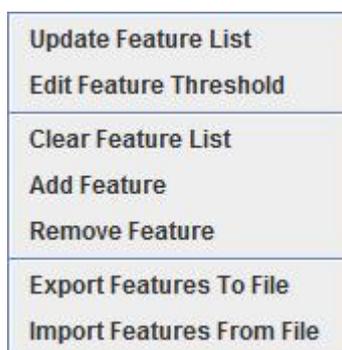


Fig. 21 Popup menu for feature tool window tab

Feature tool window tab

Feature tool window tab contains a list of potential feature points identified by users. Each row in the tab represents a feature entity which contains retention time, m/z value of the feature point and two sets of separated integers (see Fig. 22).

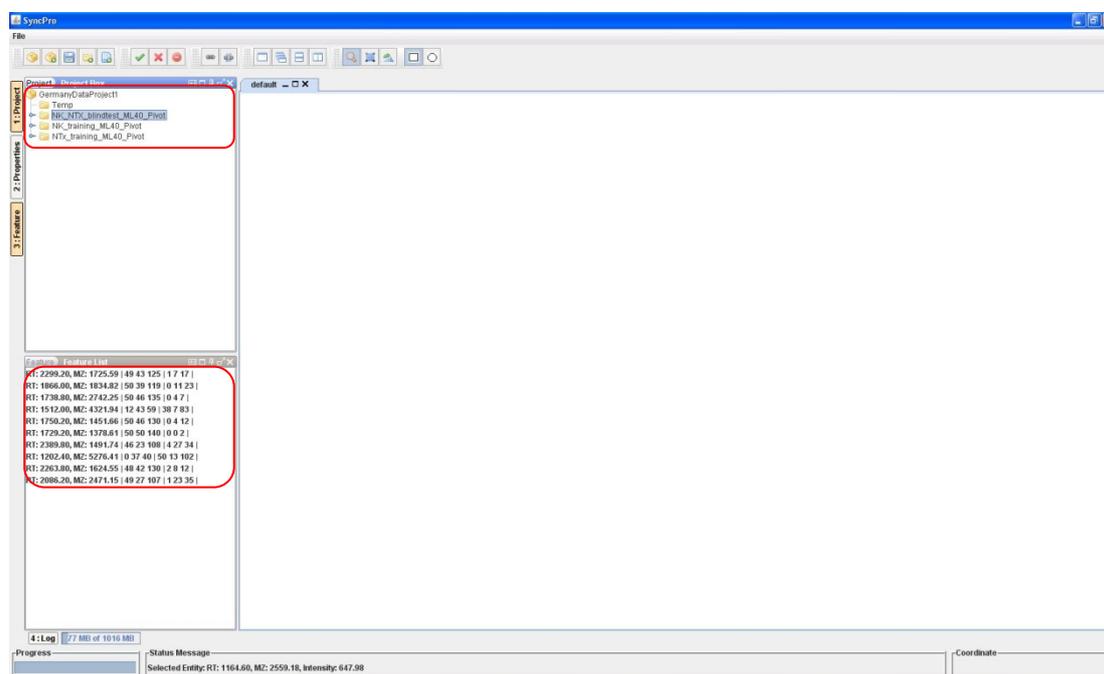


Fig. 22 A project with multiple selected features in the feature tool window tab

For a feature point and all file nodes in the current project, the first set of integers represents the number of file nodes which have the feature point (i.e. these nodes have at least one data point within the retention time and m/z threshold range specified by users). The second set of integers represents the number of file nodes which don't have the feature point. The category of each file node can be set via the "Set Diagnosis Type" option in the popup menu of the project tool window tab. The retention time and m/z threshold can be modified using the option "Edit Feature Threshold" in Fig. 21. A popup dialog will be shown for inputting new threshold values (see Fig. 23).

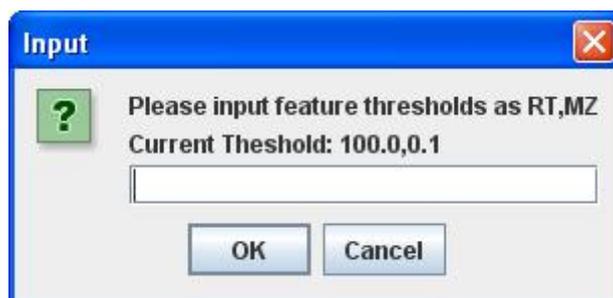


Fig. 23 Dialog for editing threshold values of feature scatter plot

Exporting feature file

1. Enable the feature tool window tab by clicking on the tab label “Feature” at the left boundary of the SyncPro program.
2. Choose the option “Export features to file” to export features to a file (see Fig. 24).

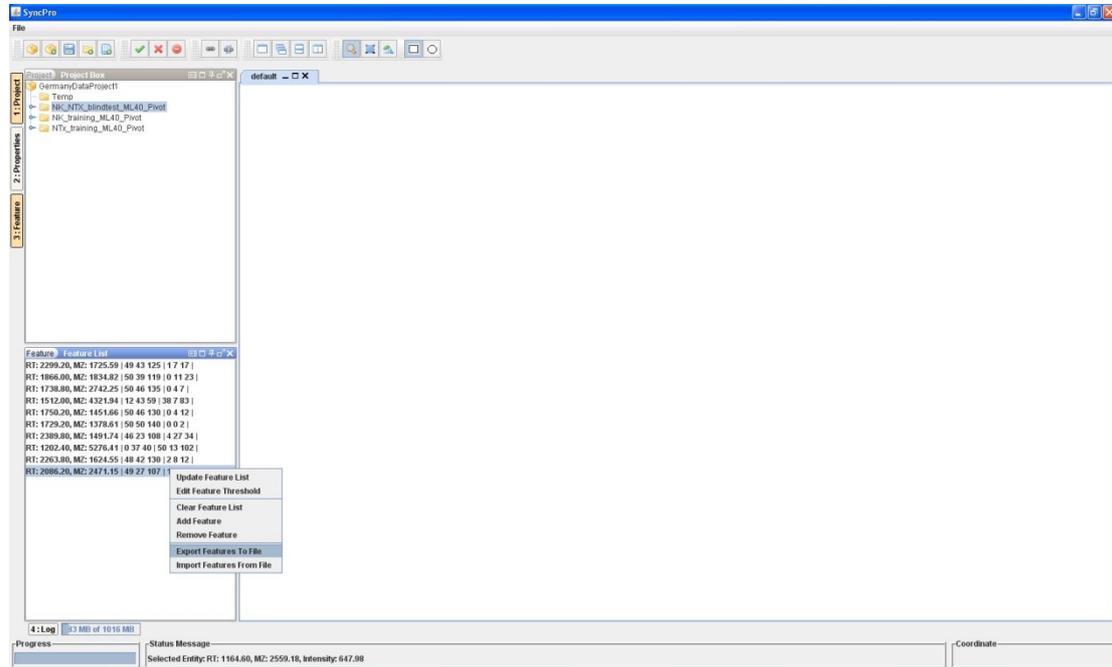


Fig. 24 Exporting a feature file

3. Select the desired directory and give a name to the feature file.
4. Click on the “Save” button in the dialog to finish the exporting process.

Importing feature file

1. Enable the feature tool window tab by clicking on the tab label “Feature” at the left boundary of the SyncPro program.
2. Choose the option “Import Features From File” to import features from a file (see Fig. 25).

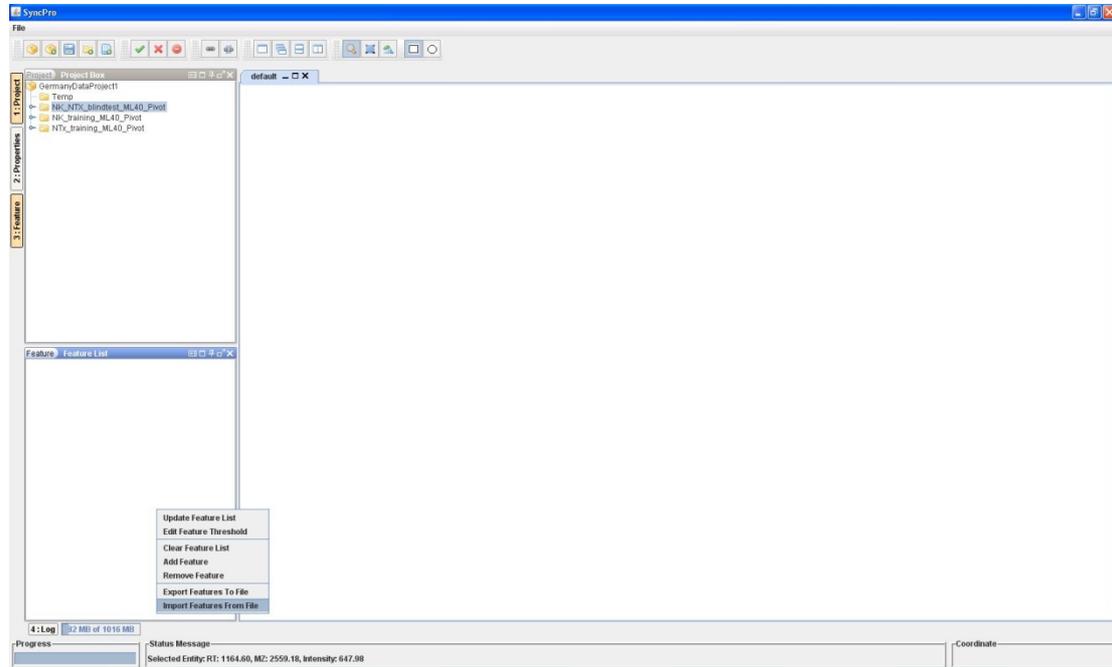


Fig. 25 Importing a feature file

3. Select the feature file in the desired directory.
4. Click on the “Open” button in the dialog to finish the importing process. SyncPro program will then import all feature points and update threshold values in the imported file.

Changing features in the scatter plot

1. Gain the keyboard focus on a feature scatter plot by clicking on any area within the plot. Then direction keys' (a set of arrow keys near the numpad) actions can be detected for exploring different features.
2. Change the feature points using direction keys of the keyboard (left arrow and right arrow for x-axis, up arrow and down arrow for y-axis).
3. Check the axis titles of the feature scatter plot to figure out which feature point is shown (see Fig. 26).

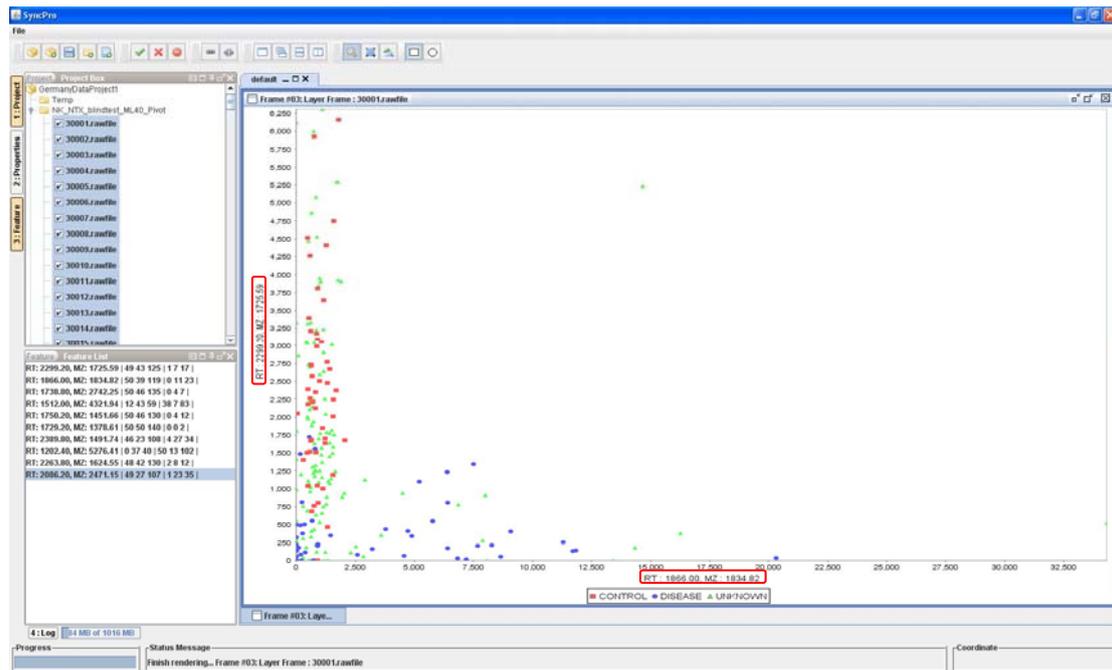


Fig. 26 A sample of feature scatter plot

Remarks:

If the feature points showing on the x-axis and y-axis are the same, then a strict line will be produced. A good feature point in this case should have a clear cut between different subsets of file nodes.

3.3. Layering and synchronization of plots

3.3.1. Layering

When dragging and dropping file nodes to the tab in the program desktop tab, users are allowed to select “Layered Frame”. All file nodes will be collectively added to the same internal frame and rendered in a descending order of sequence of file nodes in the project tree. The first file node will be the last one to be rendered.



Fig. 27 Tool bar options of layering

Making a file node visible/invisible

1. Click on any internal frame in the tab of the program desktop pane. All file nodes in the project tree having a reference to that internal frame will be highlighted.
2. Select multiple folder nodes or file nodes in the project tree by holding the “Shift” or “Ctrl” Key.
3. Click on {2} (see Fig. 27) or the option “Unselect” to make all selected nodes invisible in the corresponding frame (see Fig. 28).

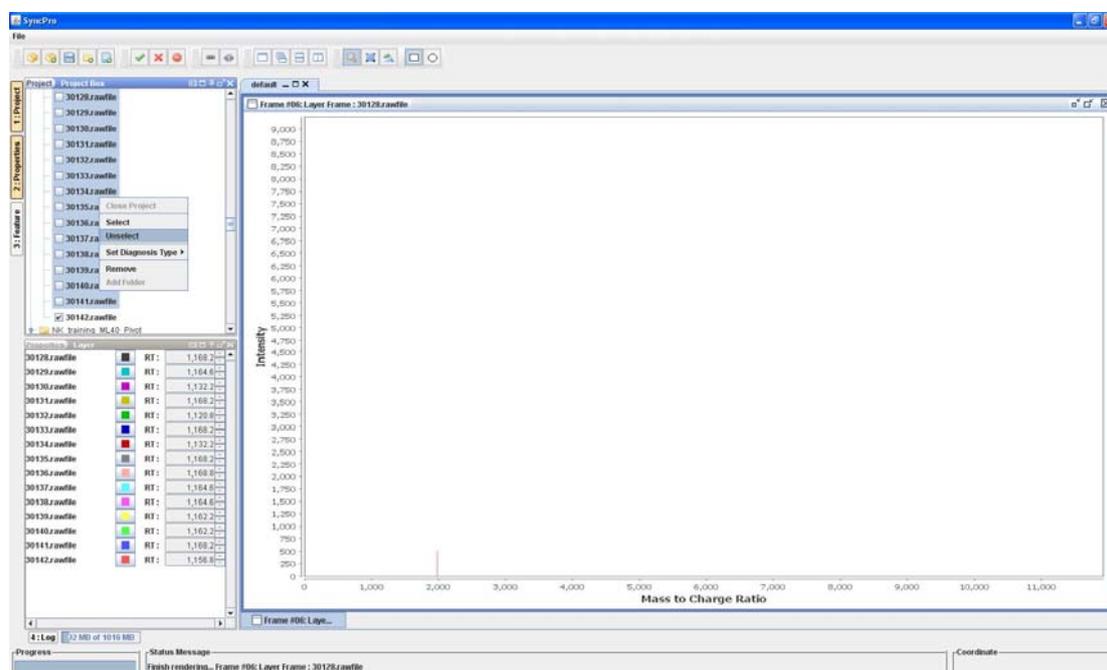


Fig. 28 Making 14 unknown samples invisible in the spectrum plot

- Click on {1} (see Fig. 27) or the option “Select” to make all selected nodes visible again in corresponding frame (see Fig. 29).

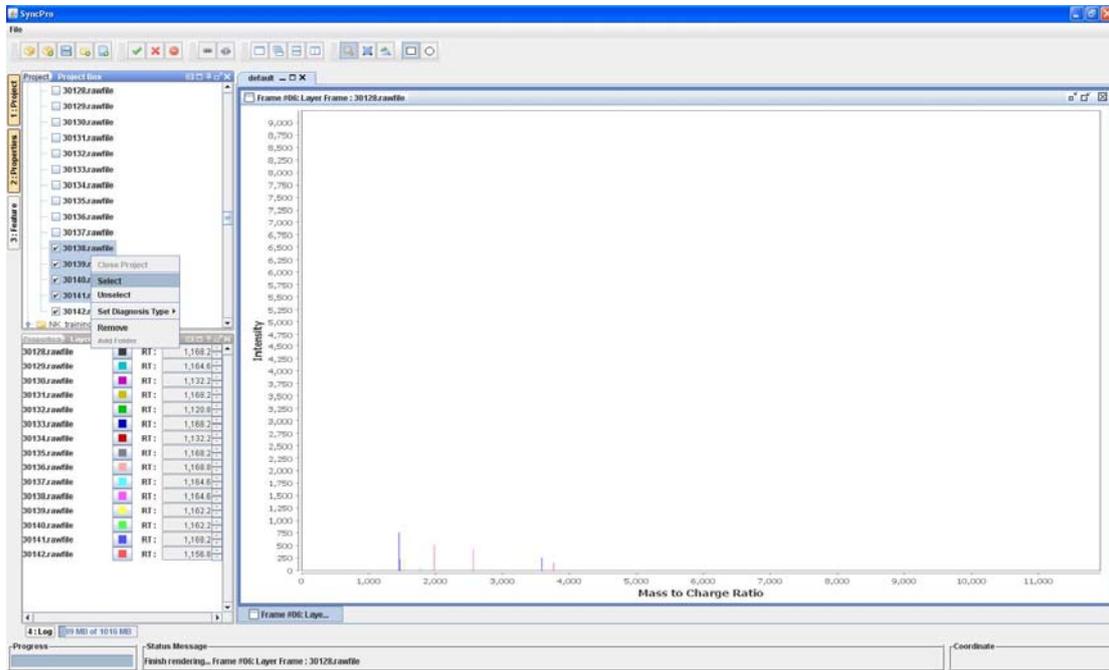


Fig. 29 Making 4 unknown samples visible in the spectrum plot

3.3.2. Synchronization

Synchronization of various plots helps to achieve a better comparative analysis of large amount of proteomics datasets.

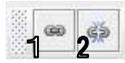


Fig. 30 Tool bar options of synchronization

Enabling/Disabling synchronization of a specific plot

1. Visualize multiple file nodes as a number of individual frames in the same tab of the program desktop pane.
2. Gain the focus on the tab by clicking on any internal frame in the tab.
3. Click on {1} (see Fig. 30) to link all internal frames in the tab.
4. Choose the desired synchronization type in some internal frames. These frames will serve as parents to trigger synchronization.
5. Manipulate parent frames to trigger desired synchronization.
6. Disable synchronization by clicking on {2} (see in Fig. 30) to break all linked frame in the current tab.

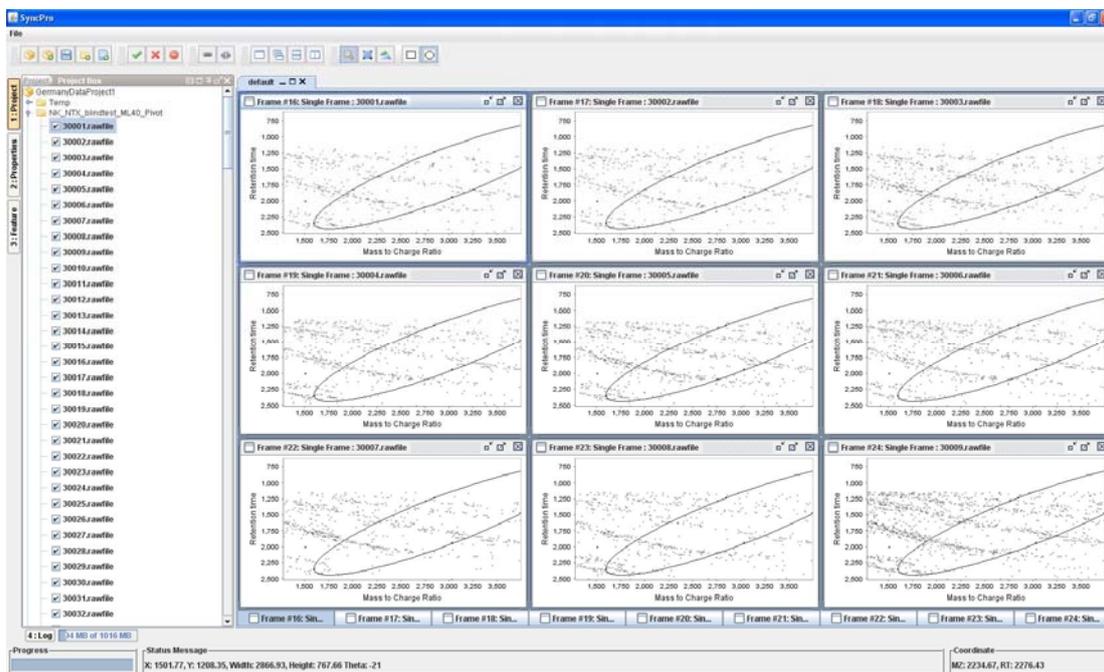


Fig. 31 Synchronization of nine internal frames for the plot axes and the selected ellipsoid windows

2D-intensity plot

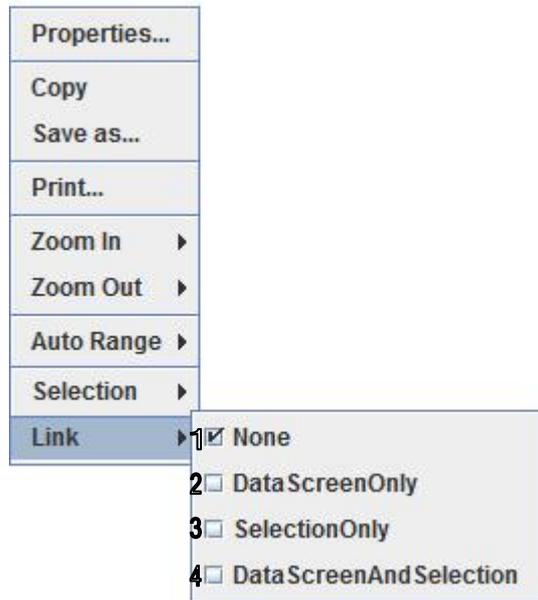


Fig. 32 Synchronization options of the 2D-intensity plot

Synchronization of 2D-intensity plot

1. None – It will not trigger any synchronization, but it will accept synchronization from others plots.
2. DataScreenOnly – It will trigger synchronization and will force plot axes of all linked plots to be the same.
3. SelectionOnly – It will trigger synchronization and all linked plots will make same selections.
4. DataScreenAndSelection – It will trigger synchronization. Both selections and plot axes of all linked plots will be synchronized.

Spectrum plot



Fig. 33 Synchronization options of the spectrum plot

Synchronization of Spectrum plot

1. None – It will not trigger any synchronization, but it will accept synchronization from other plots.
2. DomainOnly – It will trigger synchronization and will force domain axes of all linked plots to be the same.
3. RangeOnly – It will trigger synchronization and will force range axes of all linked plots to be the same.
4. DomainAndRange – It will trigger synchronization and will force both domain and range axes of all linked plots to be the same.

Feature scatter plot

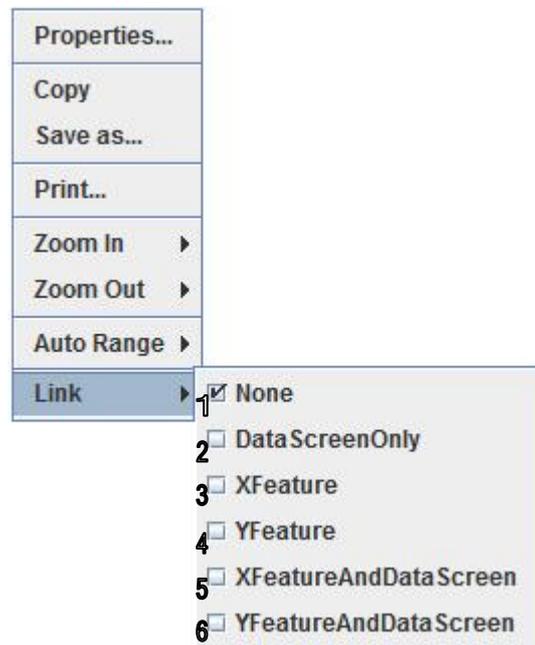


Fig. 34 Synchronization options of the feature scatter plot

Synchronization of Feature scatter plot

1. None – It will not trigger any synchronization, but it will accept synchronization from other plots.
2. DataScreenOnly – It will trigger synchronization and will force plot axes of all linked plots to be the same.
3. XFeature – It will trigger synchronization and will force the feature shown in the x axis of feature scatter plot to be the same.
4. YFeature – It will trigger synchronization and will force the feature shown in the y axis of feature scatter plot to be the same.
5. XFeatureAndDataScreen – It will trigger synchronization. The feature shown in the x axis and the plot axes will be synchronized.
6. YFeatureAndDataScreen – It will trigger synchronization. The feature shown in the y axis and the plot axes will be synchronized.