spectragui

File Data Pre-Processing MVA Data Display

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
Select Data	Select Variables	Select Filenames	Select Totalcounts	Select Samples

This tutorial contains navigation buttons that enable you to move throughout the tutorial.

Please use the navigation buttons and not the page up/page down or arrow keys to navigate through the tutorials.

This is the 'Next' button. It takes you to the next frame or stop point.

This is the 'Previous' button. It takes you to the previous frame or stop point.

This is the 'Go to frame' button. It takes you to a specified frame.

This is the 'Go to URL' button. It takes you to a website link.

Press the 'Next' button below to start this tutorial.

MATLAB 7.3.0 (R2006b)

File Edit View Graphics Debug

Shortcuts How to Add Wha

Workspace

Name

- Xdata
- Ydata
- data
- exactmass
- filenames
- labels
- loads
- model
- ndatass
- nommass
- samplenames
- scores
- totalcounts
- variance

Current Directory Workspace

Command History

%-- 10/5/10 10:04 Al

Start

spectragui

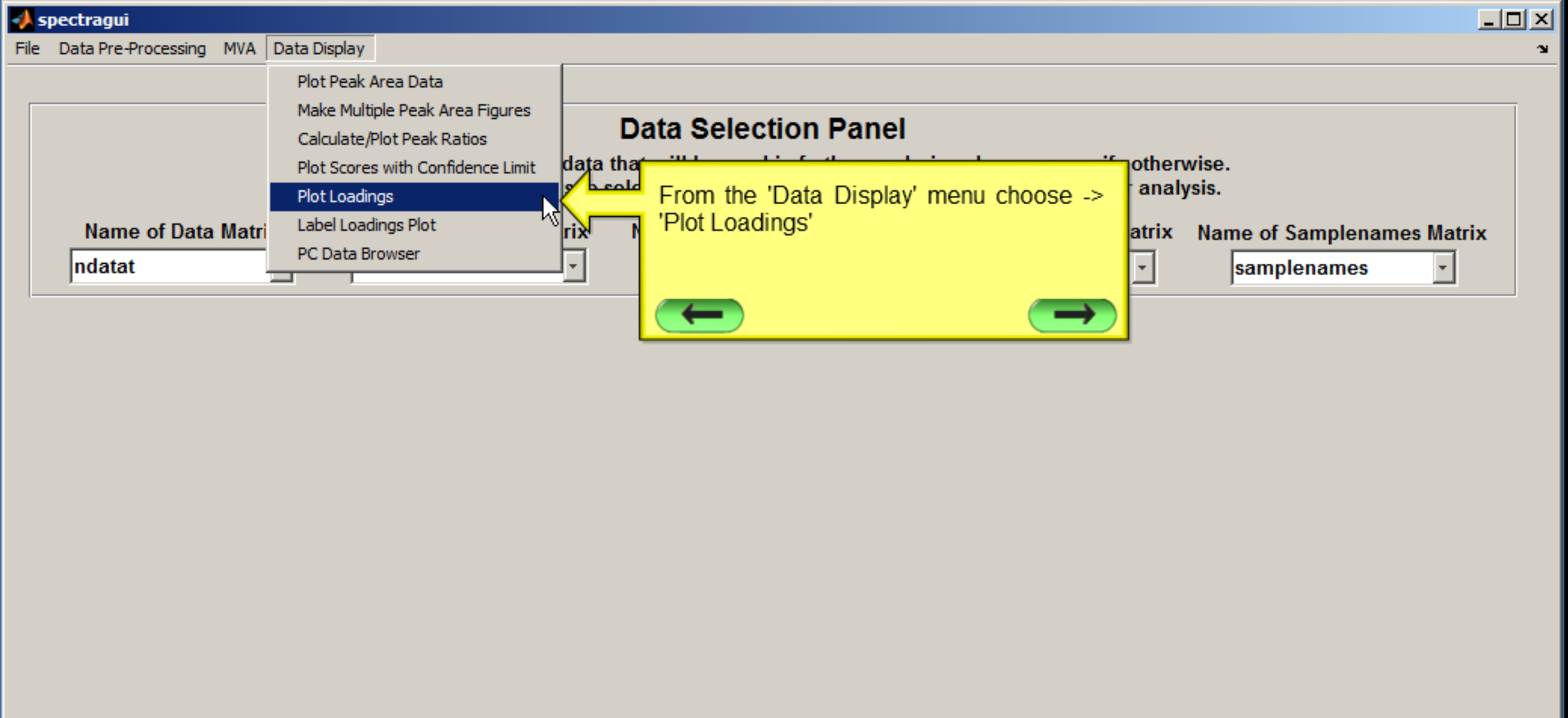
File Data Pre-Processing MVA Data Display

Raw Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	Select Samples

This tutorial will show how to create and label a loadings plot.


spectragui
File
Data Pre-Processing
MVA
Data Display
Plot Peak Area Data
Make Multiple Peak Area Figures
Calculate/Plot Peak Ratios
Plot Scores with Confidence Limit
Plot Loadings
Label Loadings Plot
PC Data Browser
Data Selection Panel
Name of Data Matri
ndatat
Name of Samplenames Matrix
samplenames
From the 'Data Display' menu choose -> 'Plot Loadings'

MATLAB 7.3.0 (R2006b)

File Edit View Graphics Debug

Shortcuts How to Add Wha

Workspace

Name

- Xdata
- Ydata
- data
- exactmass
- filenames
- labels
- loads
- model
- ndatass
- nommass
- samplenames
- scores
- totalcounts
- variance

Current Directory Workspace

Command History

%-- 10/5/10 10:04 Al

Start

spectragui

File Data Pre-Processing MVA Data Display

Raw Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	Select Samples

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
scores	loads	variance	model

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Make sure the proper data is selected and press the 'Load Selected Data' button.

PC# to plot

Plot Loads

MATLAB 7.3.0 (R2006b)

File Edit View Graphics Debug

Shortcuts How to Add Wha

Workspace

Name

- Xdata
- Ydata
- data
- exactmass
- filenames
- labels
- loads
- model
- ndatass
- nommass
- samplenames
- scores
- totalcounts
- variance

Current Directory Workspace

Command History

%-- 10/5/10 10:04 Al

Start

spectragui

File Data Pre-Processing MVA Data Display

Raw Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	Select Samples

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
scores	loads	variance	model

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings:	loads
Variables:	exactmass
% Variance:	variance

PC# to plot

Panel

Enter the PC number you want to plot the loadings for.

MATLAB 7.3.0 (R2006b)

File Edit View Graphics Debug

Shortcuts How to Add Wha

Workspace

Name

- Xdata
- Ydata
- data
- exactmass
- filenames
- labels
- loads
- model
- ndatass
- nommass
- samplenames
- scores
- totalcounts
- variance

Current Directory Workspace

Command History

%-- 10/5/10 10:04 Al

Start

spectragui

File Data Pre-Processing MVA Data Display

Raw Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	Select Samples

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
scores	loads	variance	model

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: loads
Variables: exactmass
% Variance: variance

PC# to plot

1

Plot Loads

Press the 'Plot Loads' button

MATLAB 7.3.0 (R2006b)

File Edit View Graphics Debug

Shortcuts How to Add Wha

Workspace

Name

- Xdata
- Ydata
- data
- exactmass
- filenames
- labels
- loads
- model
- ndatass
- nommass
- samplenames
- scores
- totalcounts
- variance

Current Directory Workspace

Command History

%-- 10/5/10 10:04 A

Start

spectragui

File Data Pre-Processing MVA Data Display

Raw Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	Select Samples

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
scores	loads	variance	model

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: loads
Variables: exactmass
% Variance: variance

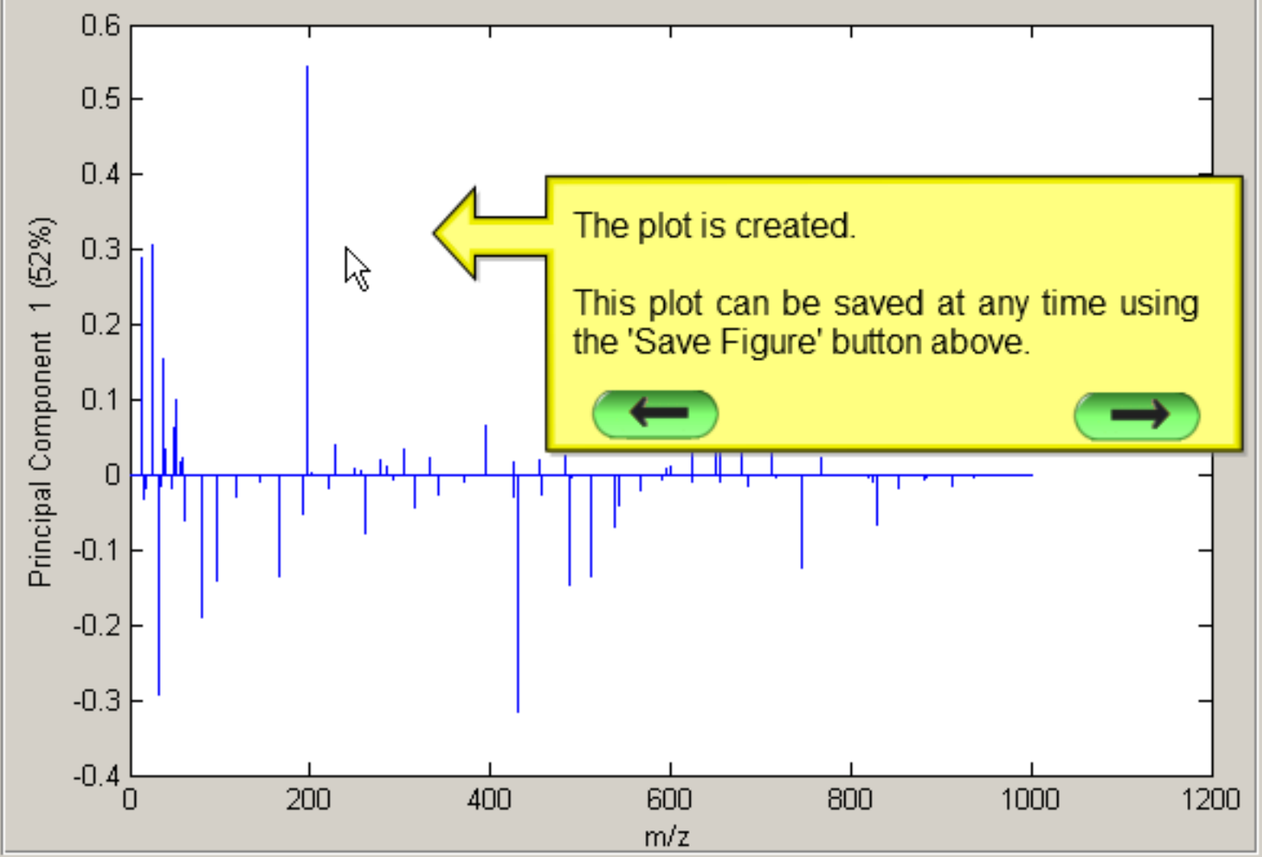
PC# to plot

1

Plot Loads

Save Figure

Close Panel



The plot is created.

This plot can be saved at any time using the 'Save Figure' button above.

MATLAB 7.3.0 (R2006b)

File Edit View Graphics Debug

Shortcuts How to Add Wha

Workspace

Name

- Xdata
- Ydata
- data
- exactmass
- filenames
- labels
- loads
- model
- ndatass
- nommass
- samplenames
- scores
- totalcounts
- variance

Current Directory Workspace

Command History

%-- 10/5/10 10:04 Al

Start

spectragui

File Data Pre-Processing MVA Data Display

- Plot Raw Data
- Make Multiple Raw Data Figures
- Plot Scores with Confidence Limit
- Plot Loadings
- Label Loadings Plot

To label the loadings plot choose 'Label Loadings Plot' from the 'Data Display' Menu.

Raw Data Selection Panel

ta that will be used in further analysis unless you specify otherwise.

analysis.

Name of Data Matrix: ndatass

Name of Variable Matrix: exactmass

Name of Samplenames Matrix: Select Samples

MVA

Name of Scores Matrix: scores

Name of Loadings Matrix: loads

Name of % Variance Matrix: variance

Name of Model Matrix: model

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

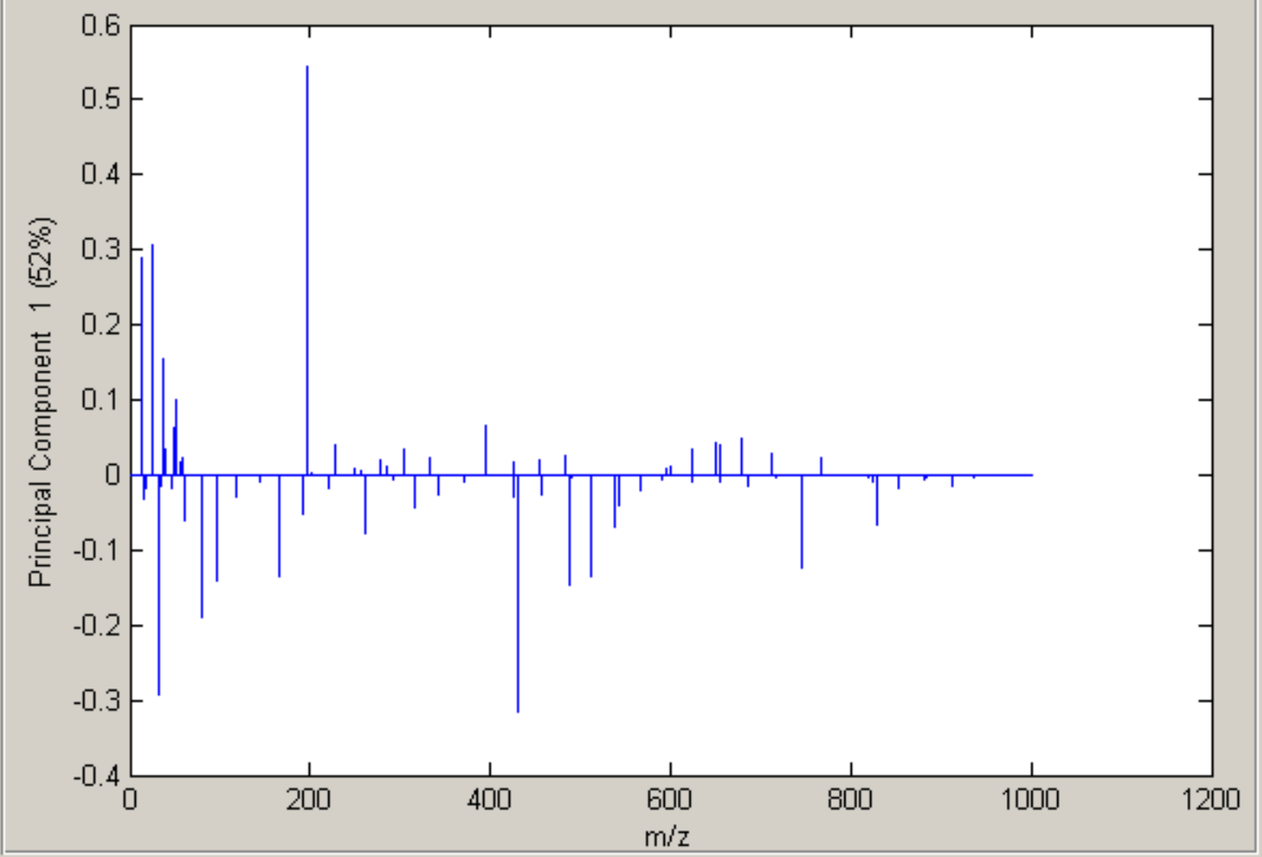
Loadings: loads
Variables: exactmass
% Variance: variance

PC# to plot: 1

Plot Loads

Save Figure

Close Panel



MATLAB 7.3.0 (R2006b)

File Edit View Graphics Debug

Shortcuts How to Add Wha

Workspace

Name

- Xdata
- Ydata
- data
- exactmass
- filenames
- labels
- loads
- model
- ndatass
- nommass
- samplenames
- scores
- totalcounts
- variance

Current Directory Workspace

Command History

%-- 10/5/10 10:04 Al

Start

spectragui

File Data Pre-Processing MVA Data Display

Raw Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	Select Samples

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
scores	loads	variance	model

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: loads
Variables: exactmass
% Variance: variance

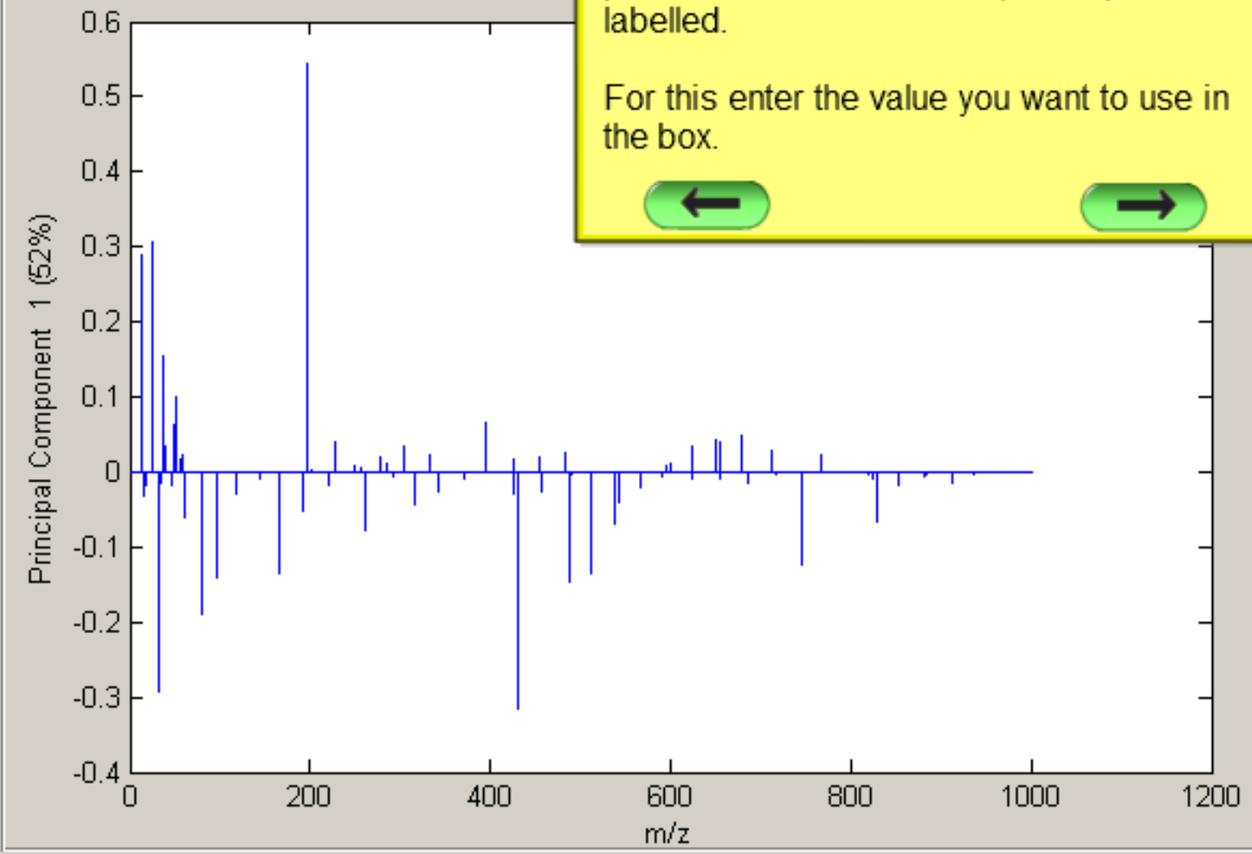
PC# to plot

1

Plot Loads

This dialog will allow you to label all loadings above a given absolute value. All peaks above this value (+ or -) will be labelled.

For this enter the value you want to use in the box.



Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Creat Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Turn Selection Mode ON/OFF

OFF

Custom Labels to use

Choose Peaks

Label Custom

Close Panel

MATLAB 7.3.0 (R2006b)

File Edit View Graphics Debug

Shortcuts How to Add Wha

Workspace

Name

- Xdata
- Ydata
- data
- exactmass
- filenames
- labels
- loads
- model
- ndatass
- nommass
- samplenames
- scores
- totalcounts
- variance

Current Directory Workspace

Command History

%-- 10/5/10 10:04 Al

Start

spectragui

File Data Pre-Processing MVA Data Display

Raw Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	Select Samples

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
scores	loads	variance	model

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

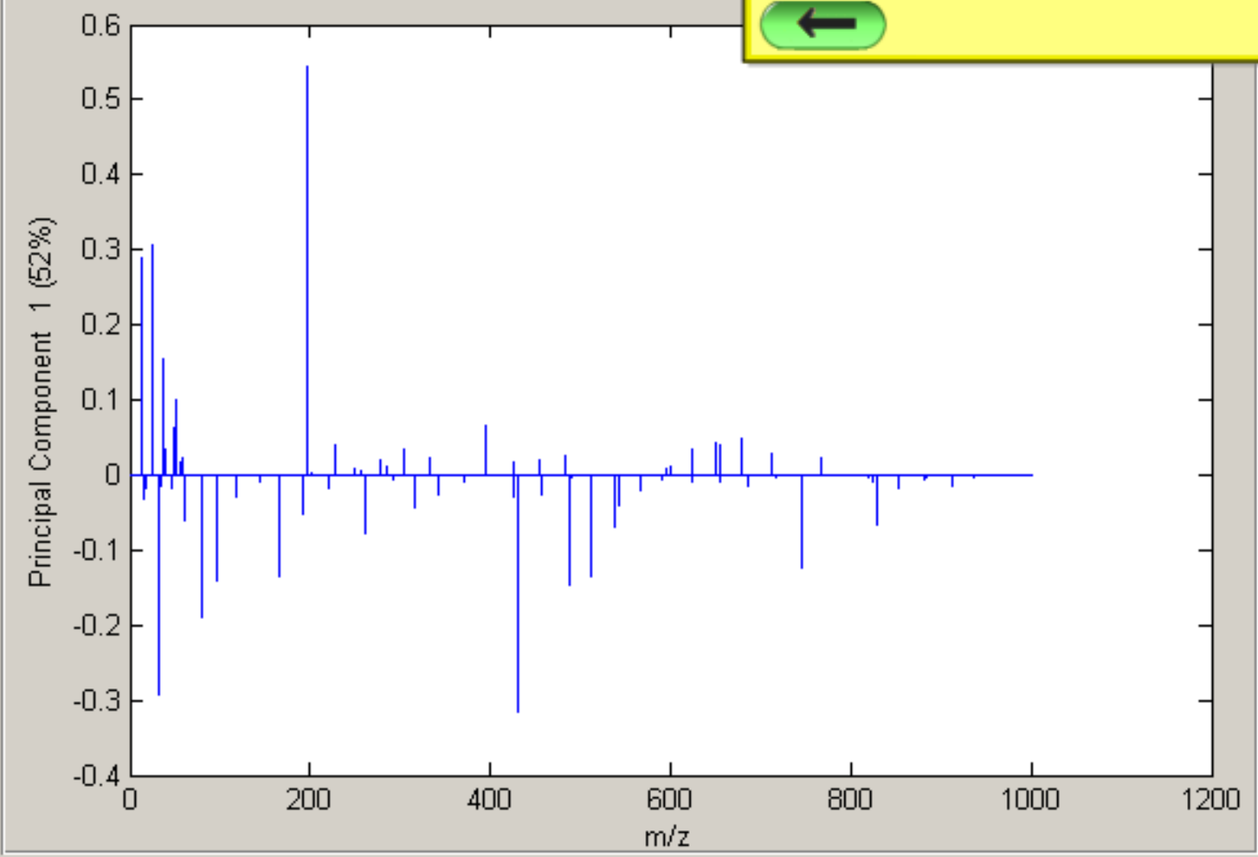
Loadings: loads
Variables: exactmass
% Variance: variance

PC# to plot

1

Plot Loads

Save Fig



And press the 'Label Threshold' button.

Label Loadings

Label all peaks above a threshold value.

Label Peaks

.1

Label Threshold

Create Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Turn Selection Mode ON/OFF

OFF

Custom Labels to use

Choose Peaks

Label Custom

Close Panel

MATLAB 7.3.0 (R2006b)

File Edit View Graphics Debug

Shortcuts How to Add Wha

Workspace

Name

- Xdata
- Ydata
- data
- exactmass
- filenames
- labels
- loads
- model
- ndatass
- nommass
- samplenames
- scores
- totalcounts
- variance

Current Directory Workspace

Command History

%-- 10/5/10 10:04 A

Start

spectragui

File Data Pre-Processing MVA Data Display

Raw Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	Select Samples

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
scores	loads	variance	model

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: loads
Variables: exactmass
% Variance: variance

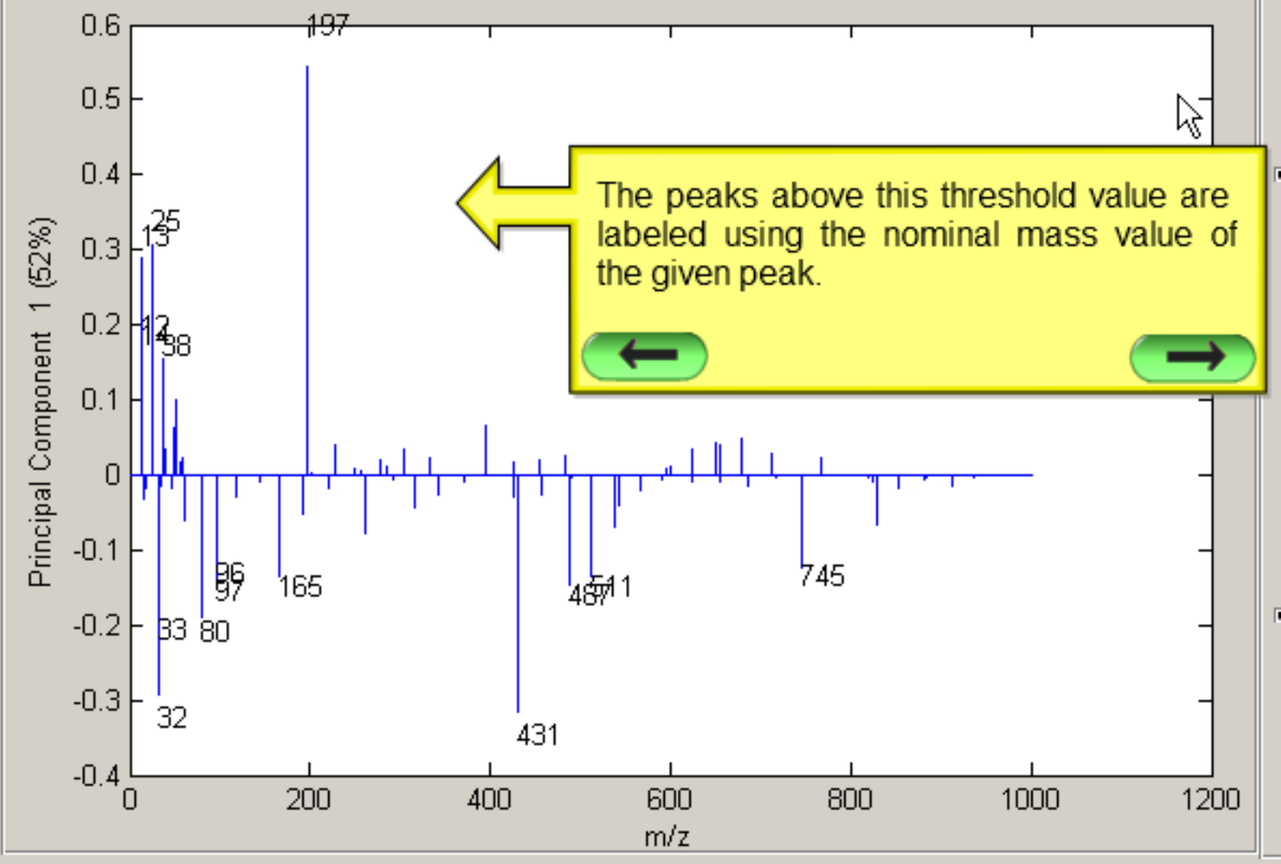
PC# to plot

1

Plot Loads

Save Figure

Close Panel



The peaks above this threshold value are labeled using the nominal mass value of the given peak.

Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

.1

Label Threshold

Creat Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Turn Selection Mode ON/OFF

OFF

Custom Labels to use

Choose Peaks

Label Custom

Close Panel

MATLAB 7.3.0 (R2006b)

File Edit View Graphics Debug

Shortcuts How to Add Wha

Workspace

Name

- Xdata
- Ydata
- data
- exactmass
- filenames
- labels
- loads
- model
- ndatass
- nommass
- samplenames
- scores
- totalcounts
- variance

Current Directory Workspace

Command History

%-- 10/5/10 10:04 A

Start

spectragui

File Data Pre-Processing MVA Data Display

Raw Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	Select Samples

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
scores	loads	variance	model

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: loads
Variables: exactmass
% Variance: variance

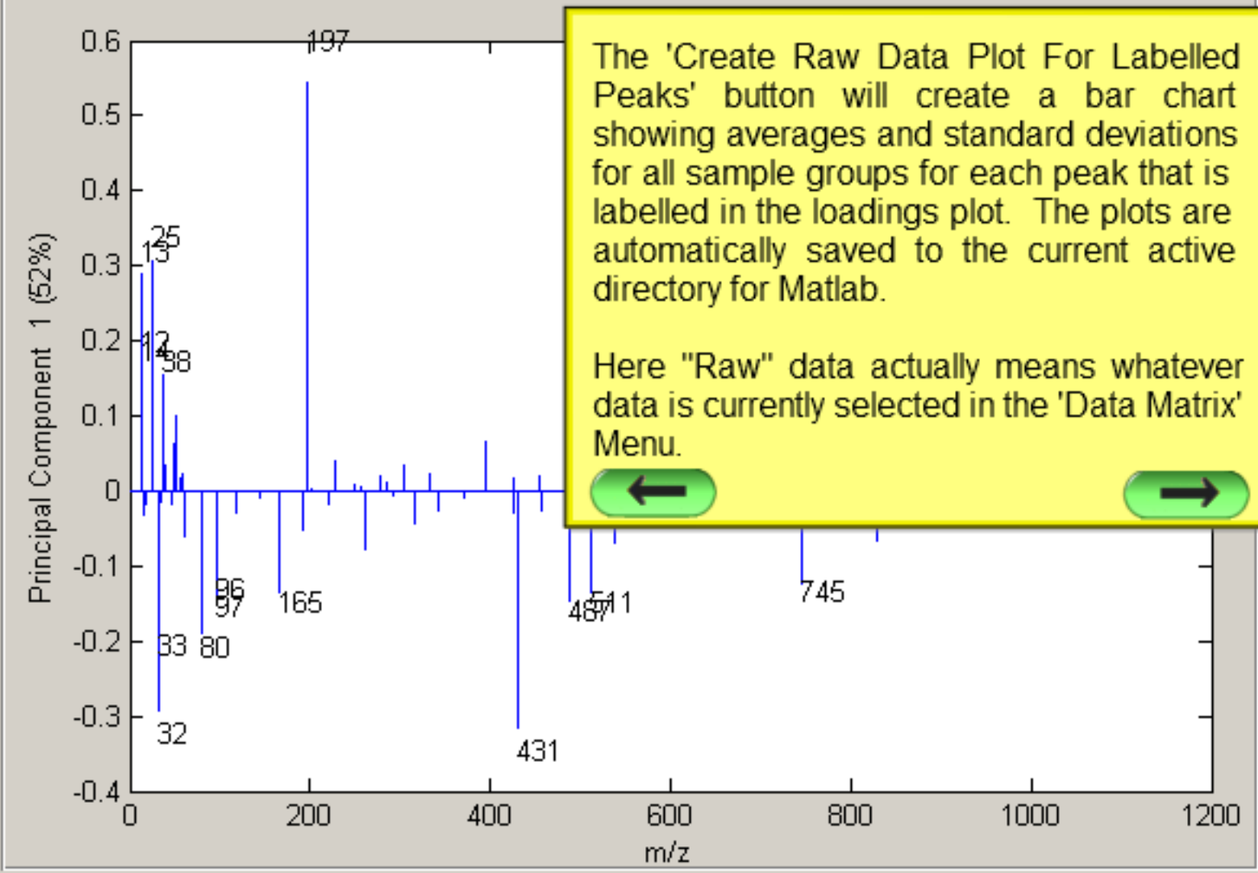
PC# to plot

1

Plot Loads

Save Figure

Close Panel



The 'Create Raw Data Plot For Labelled Peaks' button will create a bar chart showing averages and standard deviations for all sample groups for each peak that is labelled in the loadings plot. The plots are automatically saved to the current active directory for Matlab.

Here "Raw" data actually means whatever data is currently selected in the 'Data Matrix' Menu.

Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

.1

Label Threshold

Creat Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Turn Selection Mode ON/OFF

OFF

Custom Labels to use

Choose Peaks

Label Custom

Close Panel

MATLAB 7.3.0 (R2006b)

File Edit View Graphics Debug

Shortcuts How to Add Wha

Workspace

Name

- Xdata
- Ydata
- data
- exactmass
- filenames
- labeledpeaks
- labels
- loads
- model
- ndatass
- nommass
- samplenames
- scores
- totalcounts
- variance

Current Directory | Workspace

Command History

%-- 10/5/10 10:04 A

Start

spectragui

work

File Edit View Favorites Tools Help

Back | Search | Folders

Address C:\Program Files\MATLAB\R2006b\work | Go

Folders

- MDL ISIS Draw 2.5
- Messenger
- Microsoft ActiveSync
- microsoft frontpage
- Microsoft Office
- Microsoft Silverlight
- Microsoft Visual Studio
- MKS Toolkit
- Molecular Fragment Calculator
- Molecular Weight Calculator
- Movie Maker
- Mozilla Firefox
- Mozilla Thunderbird
- MSBuild
- MSECache
- MSN
- MSN Gaming Zone
- NetMeeting
- Outlook Express
- PDFCreator
- Pidgin
- PyChem
- QuickTime
- Realtek
- Realtek AC97
- Reference Assemblies
- Roxio
- Scribus 1.3.3.14
- SigmaTel
- Skype
- Sophos
- Sun
- SurfaceSpectra
- Taskbar Shuffle
- Uninstall Information

The figures are saved to the currently active Matlab directory.

Name	Size	Type	Date Modified
helpsubspace.mat	32 KB	MATLAB data file	4/29/2010 4:10 PM
H1.mat	5,572 KB	MATLAB data file	3/19/2010 3:47 PM
filenames.mat	1 KB	MATLAB data file	7/23/2010 3:02 PM
fakeimagespectradata.mat	1,988 KB	MATLAB data file	1/4/2010 4:48 PM
dnaproteinnegdataall.mat	99 KB	MATLAB data file	3/19/2010 12:20 PM
c1211.mat	5,377 KB	MATLAB data file	5/14/2010 3:57 PM
allhomoposdataDNAIgG.mat	114 KB	MATLAB data file	3/2/2010 1:48 PM
ABCF6 with C6-6.mat	204 KB	MATLAB data file	8/25/2009 10:15 AM
100721.mat	638 KB	MATLAB data file	7/26/2010 9:04 AM
scoresplot.jpg	52 KB	JPEG Image	10/5/2010 1:49 PM
745.jpg	41 KB	JPEG Image	10/5/2010 1:50 PM
511.jpg	43 KB	JPEG Image	10/5/2010 1:50 PM
487.jpg	42 KB	JPEG Image	10/5/2010 1:50 PM
431.jpg	43 KB	JPEG Image	10/5/2010 1:50 PM
197.jpg	57 KB	JPEG Image	10/5/2010 1:50 PM
165.jpg	43 KB	JPEG Image	10/5/2010 1:50 PM
97.jpg	46 KB	JPEG Image	10/5/2010 1:50 PM
96.jpg	43 KB	JPEG Image	10/5/2010 1:50 PM
80.jpg	52 KB	JPEG Image	10/5/2010 1:50 PM
38.jpg	56 KB	JPEG Image	10/5/2010 1:50 PM
33.jpg	59 KB	JPEG Image	10/5/2010 1:50 PM
32.jpg	56 KB	JPEG Image	10/5/2010 1:50 PM
25micronScan3micronfeatures...	257 KB	JPEG Image	9/28/2010 2:07 PM
25.jpg	63 KB	JPEG Image	10/5/2010 1:50 PM
14.jpg	61 KB	JPEG Image	10/5/2010 1:50 PM
13.jpg	63 KB	JPEG Image	10/5/2010 1:50 PM
12.jpg	57 KB	JPEG Image	10/5/2010 1:50 PM
test.bif6	2,561 KB	BIF6 File	7/30/2010 4:07 PM
test2.bif6	38,403 KB	BIF6 File	10/5/2010 11:01 AM
51000_01.BIF6	38,403 KB	BIF6 File	10/1/2010 2:22 PM
25500_01.BIF6	38,403 KB	BIF6 File	10/4/2010 12:42 PM
25100_01.BIF6	38,403 KB	BIF6 File	10/4/2010 12:34 PM
5100_06.BIF6	13,313 KB	BIF6 File	10/4/2010 1:34 PM
5100_01.BIF6	38,403 KB	BIF6 File	10/4/2010 12:49 PM
1100_06.BIF6	13,313 KB	BIF6 File	10/4/2010 1:28 PM
1100_02.BIF6	38,403 KB	BIF6 File	10/4/2010 12:16 PM
TIMAGE.BIF	8,580 KB	BIF File	4/29/2010 2:15 PM
TESTP04.bif	77,961 KB	BIF File	7/16/2010 7:57 AM
S1200_03.BIF	10,114 KB	BIF File	9/9/2010 3:53 PM
S1200_01.BIF	10,114 KB	BIF File	9/9/2010 3:47 PM

Matrix

-0.4

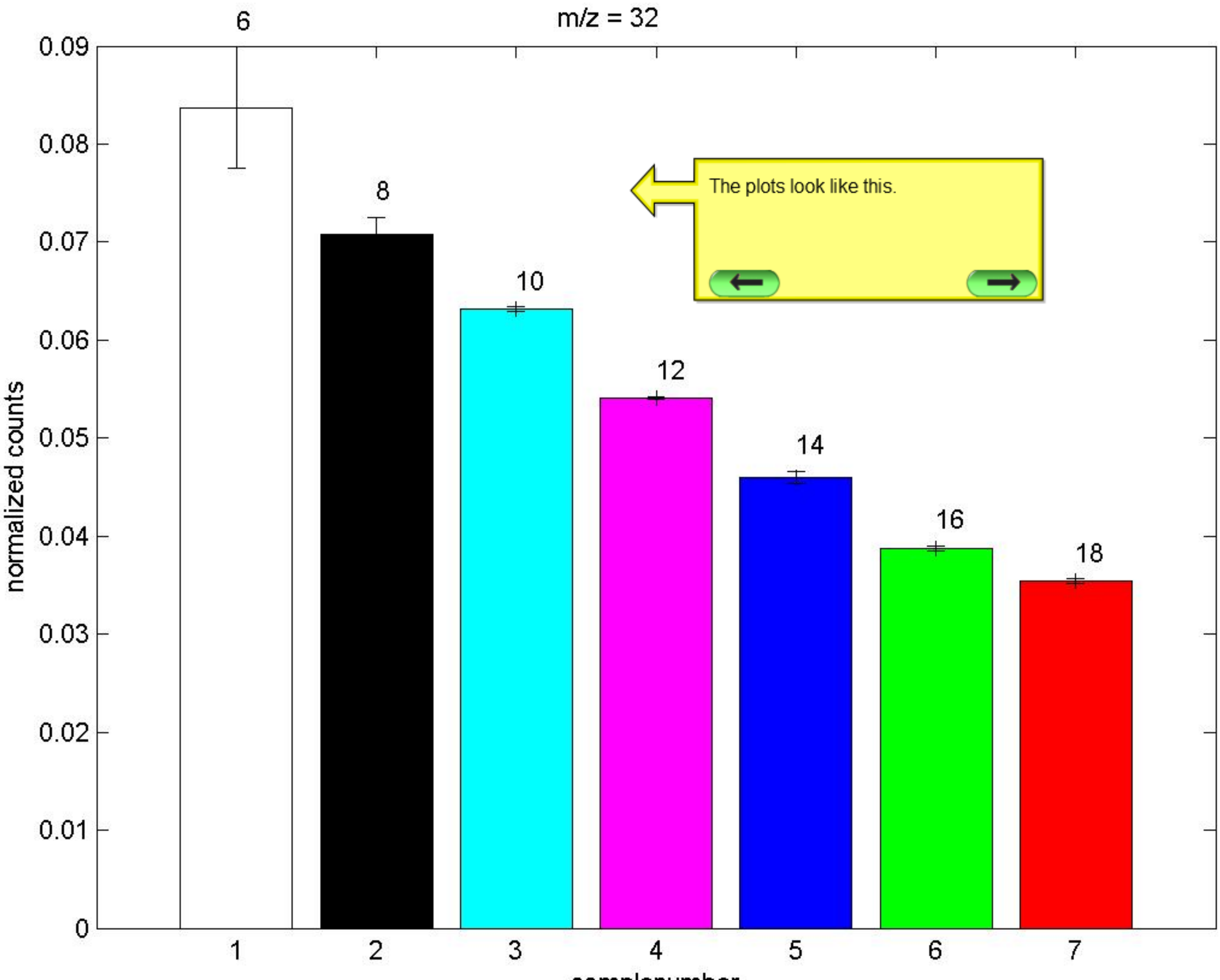
0 200 400 600 800 1000 1200

m/z

32.jpg - IrfanView

File Edit Image Options View Help

8/35



spectragui

File Data Pre-Processing MVA Data Display extra

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	samplenames

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
newscores	newloads	newvar	newmodel

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: newloads
Variables: exactmass
% Variance: newvar

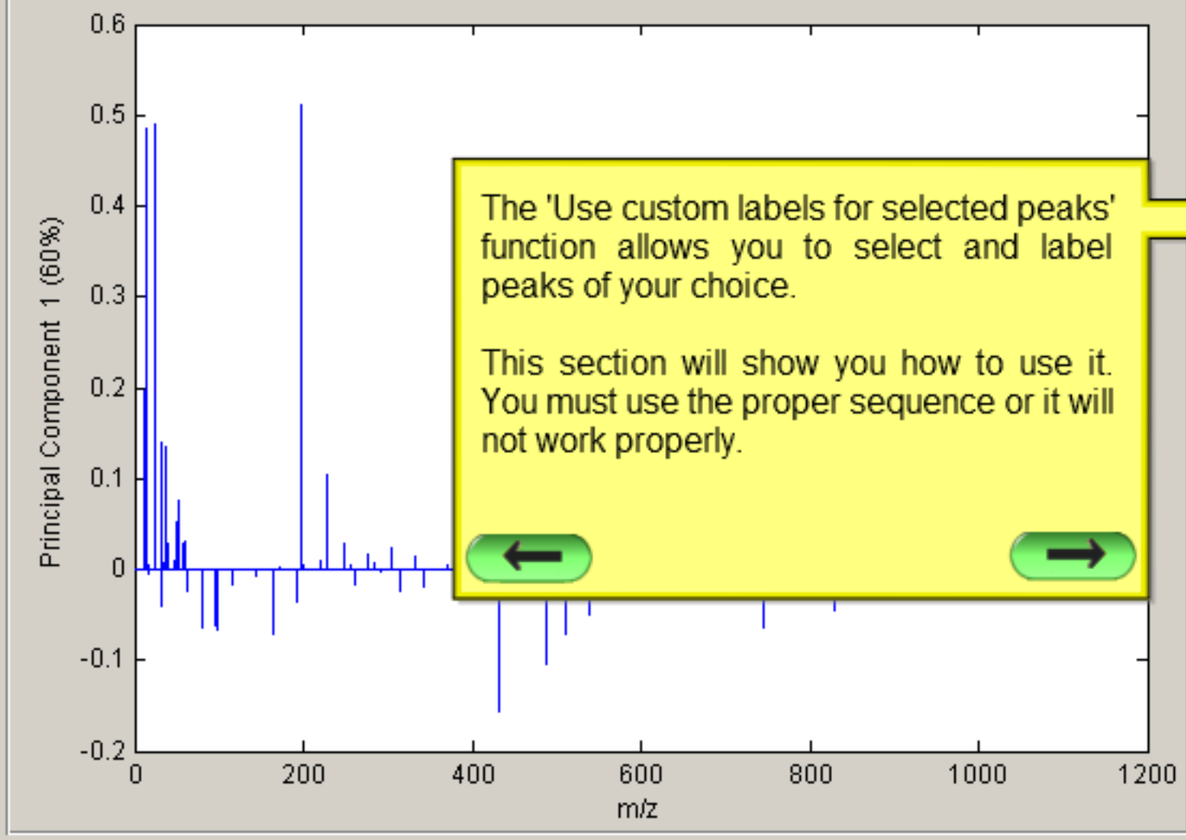
PC# to plot

1

Plot Loads

Save Figure

Close Panel



The 'Use custom labels for selected peaks' function allows you to select and label peaks of your choice.

This section will show you how to use it. You must use the proper sequence or it will not work properly.

Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Creat Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

Choose Peaks

Label Custom

Close Panel

spectragui

File Data Pre-Processing MVA Data Display extra

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	samplenames

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
newscores	newloads	newvar	newmodel

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: newloads
Variables: exactmass
% Variance: newvar

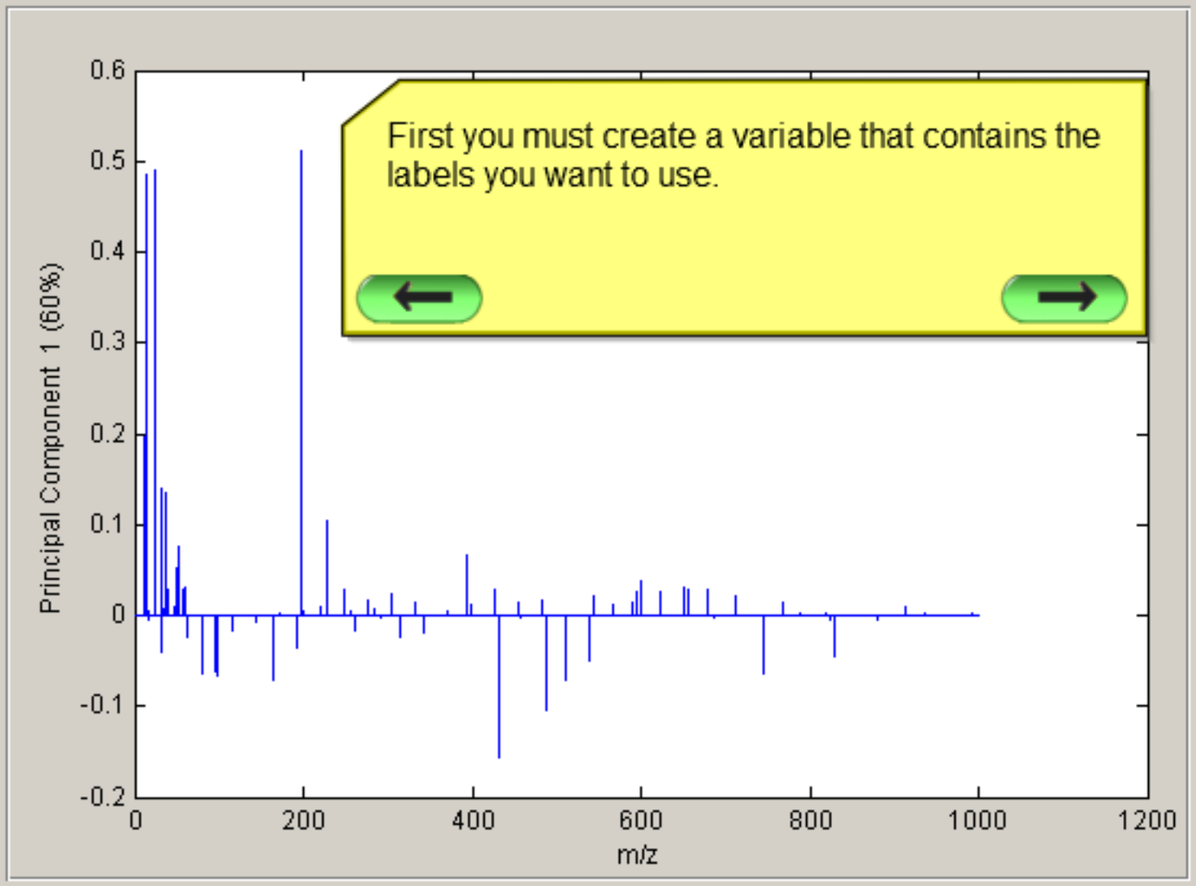
PC# to plot

1

Plot Loads

Save Figure

Close Panel



Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Creat Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

Choose Peaks

Label Custom

Close Panel

Current Folder: C:\Documents and Settings\graham\My Documents\MATLAB

Command Window

```
>> spectragui
>>
```

Because of how Matlab handles text, all the labels must all have the same number of characters. You can use spaces if the labels you want to use have different lengths.

The general format is:
variablename=['label1'; 'label2'; 'label3';...'labeln']

data to plot

	Min	Max
	1	1478
	1.941...	0.15
	-0.6479	0.56
	-1.35...	5.74
	1	1.63
	1340207	2519

Current Folder: C:\Documents and Settings\graham\My Documents\MATLAB

data to plot

	Min	Max
	1	1478
	1.941...	0.15
	-0.6479	0.56
	-1.35...	5.74
	1	1.63
	1340207	2519

Command Window

```
>> spectragui
>> customlabels=['These';'Are  ';'Big  ';'Peaks'];
```

Note the spaces to keep the labels the same length.

Current Folder: C:\Documents and Settings\graham\My Documents\MATLAB

Command Window

```
>> spectragui
>> customlabels=['These';'Are  ';'Big  ';'Peaks'];
>>
```

Press <enter> to save the new variable to the workspace.

data to plot

	Min	Max
	1	1478
	1.941...	0.15
	-0.6479	0.56
	-1.35...	5.74
	1	1.63
	1340207	2519

Current Folder: C:\Documents and Settings\graham\My Documents\MATLAB

data to plot

	Min	Max
	1	1478
	1.941...	0.15
	-0.6479	0.56
	-1.35...	5.74
	1	1.63
	1340207	2519

Command Window

```
>> spectragui
>> customlabels=['These';'Are  ';'Big  ';'Peaks'];
>> customlabels

customlabels =

These
Are
Big
Peaks

>>
```

The new labels variable is created.

spectragui

File Data Pre-Processing MVA Data Display extra

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix: ndatass
Name of Variable Matrix: exactmass
Name of Filename Matrix: filenames
Name of Totalcounts Matrix: totalcounts
Name of Samplenames Matrix: samplenames

MVA Data Selection Panel

Name of Scores Matrix: newscores
Name of Loadings Matrix: newloads
Name of % Variance Matrix: newvar
Name of Model Matrix: newmodel

Plot Loadings

Load Selected Data

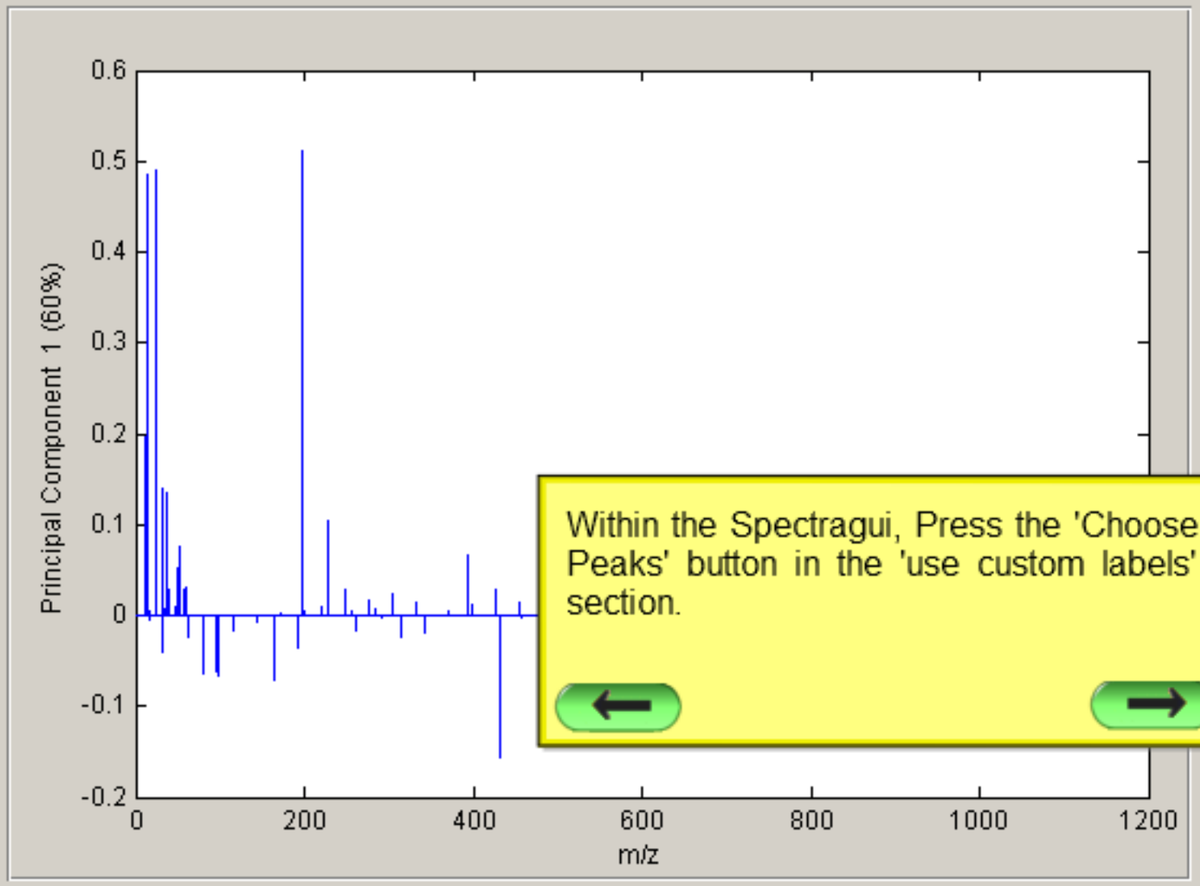
Load Selected Data

Loaded Data

Loadings: newloads
Variables: exactmass
% Variance: newvar

PC# to plot: 1

Plot Loads | Save Figure | Close Panel



Within the Spectragui, Press the 'Choose Peaks' button in the 'use custom labels' section.

Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Creat Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

Choose Peaks

Label Custom

Close Panel

spectragui

File Data Pre-Processing MVA Data Display extra

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	samplenames

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
newscores	newloads	newvar	newmodel

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: newloads
Variables: exactmass
% Variance: newvar

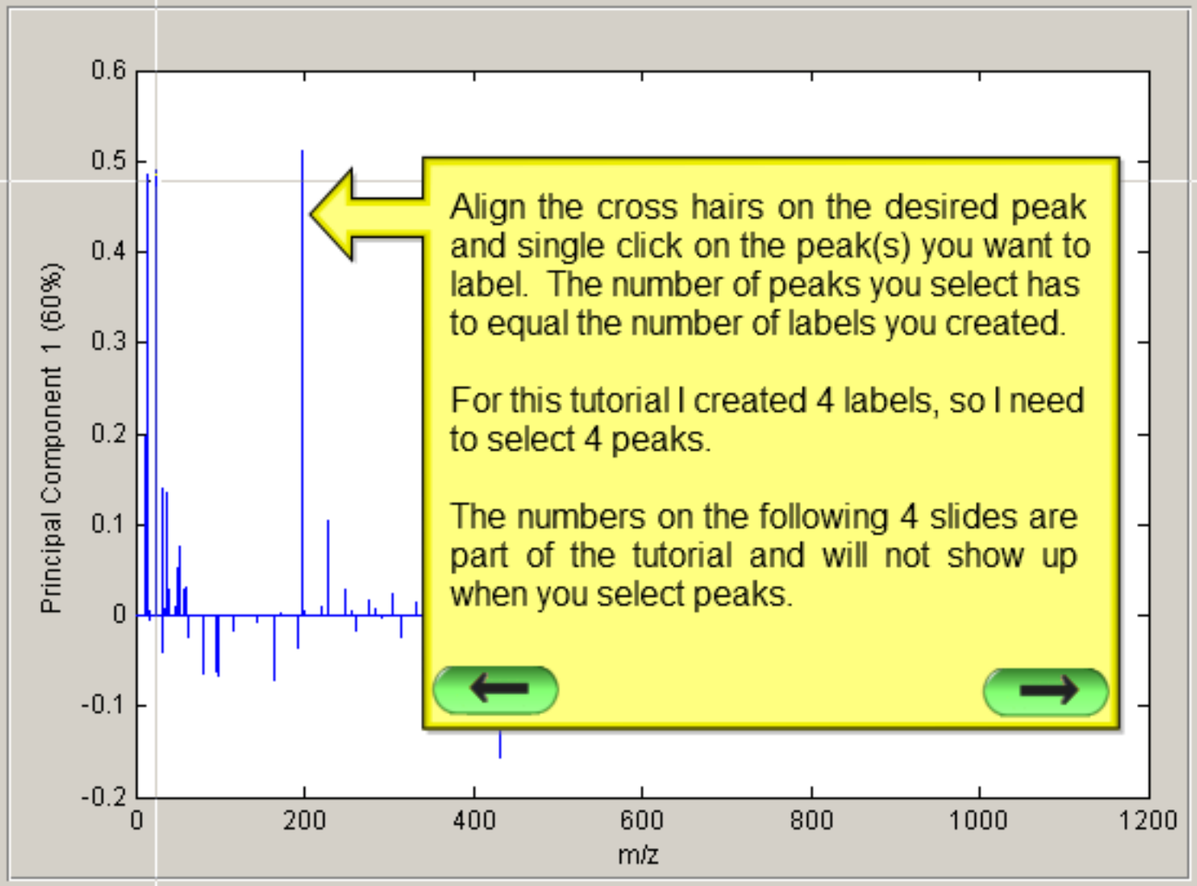
PC# to plot

1

Plot Loads

Save Figure

Close Panel



Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Creat Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

Choose Peaks

Label Custom

Close Panel

spectragui

File Data Pre-Processing MVA Data Display extra

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	samplenames

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
newscores	newloads	newvar	newmodel

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: newloads
Variables: exactmass
% Variance: newvar

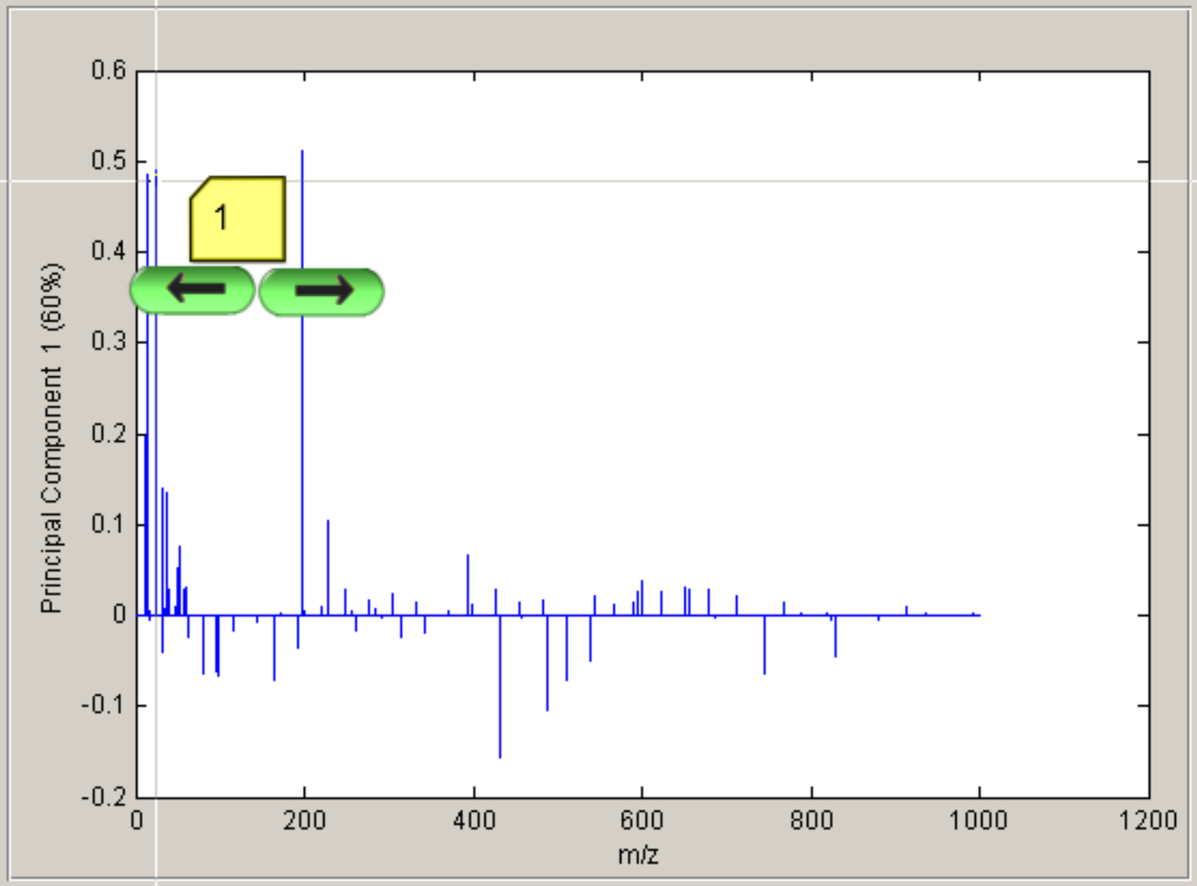
PC# to plot

1

Plot Loads

Save Figure

Close Panel



Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Creat Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

Choose Peaks

Label Custom

Close Panel

spectragui

File Data Pre-Processing MVA Data Display extra

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	samplenames

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
newscores	newloads	newvar	newmodel

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: newloads
Variables: exactmass
% Variance: newvar

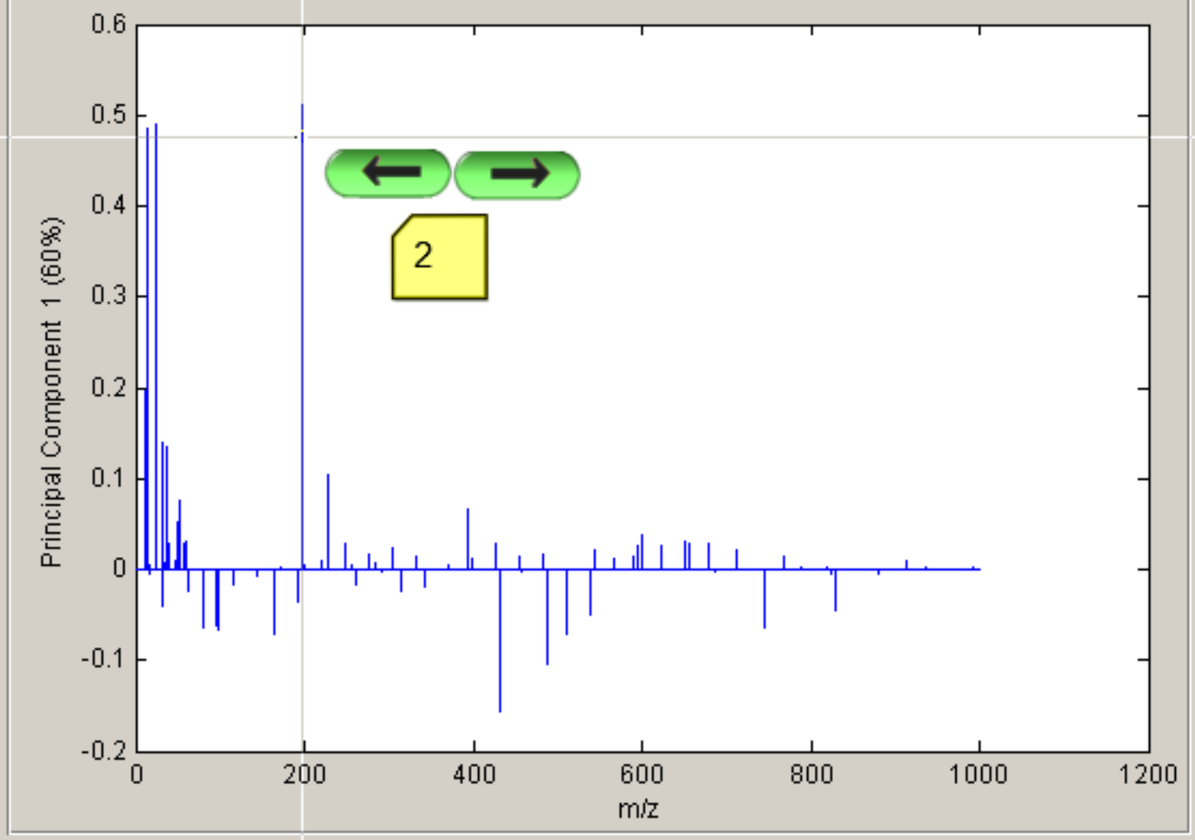
PC# to plot

1

Plot Loads

Save Figure

Close Panel



Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Creat Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

Choose Peaks

Label Custom

Close Panel

spectragui

File Data Pre-Processing MVA Data Display extra

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	samplenames

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
newscores	newloads	newvar	newmodel

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: newloads
Variables: exactmass
% Variance: newvar

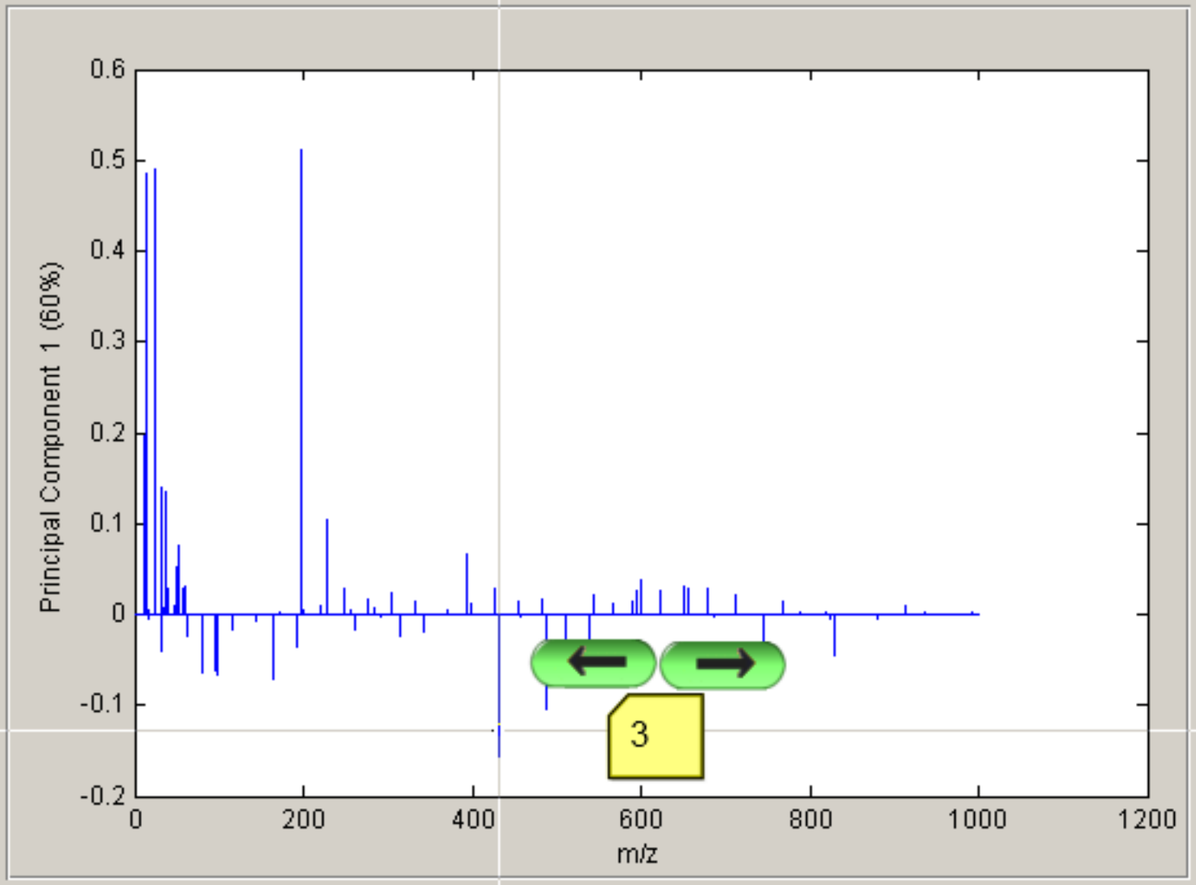
PC# to plot

1

Plot Loads

Save Figure

Close Panel



Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Creat Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

Choose Peaks

Label Custom

Close Panel

spectragui

File Data Pre-Processing MVA Data Display extra

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	samplenames

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
newscores	newloads	newvar	newmodel

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: newloads
Variables: exactmass
% Variance: newvar

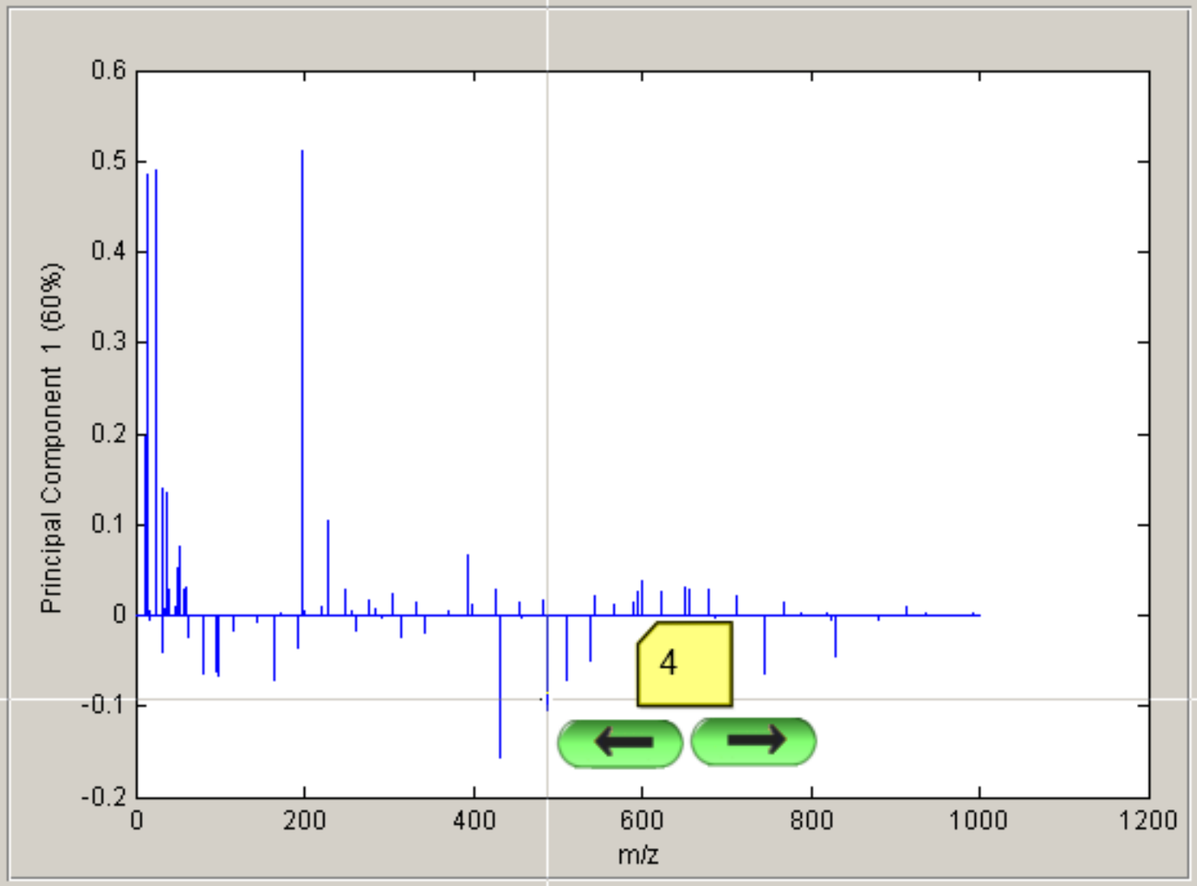
PC# to plot

1

Plot Loads

Save Figure

Close Panel



Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Creat Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

Choose Peaks

Label Custom

Close Panel

spectragui

File Data Pre-Processing MVA Data Display extra

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	samplenames

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
newscores	newloads	newvar	newmodel

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: newloads
Variables: exactmass
% Variance: newvar

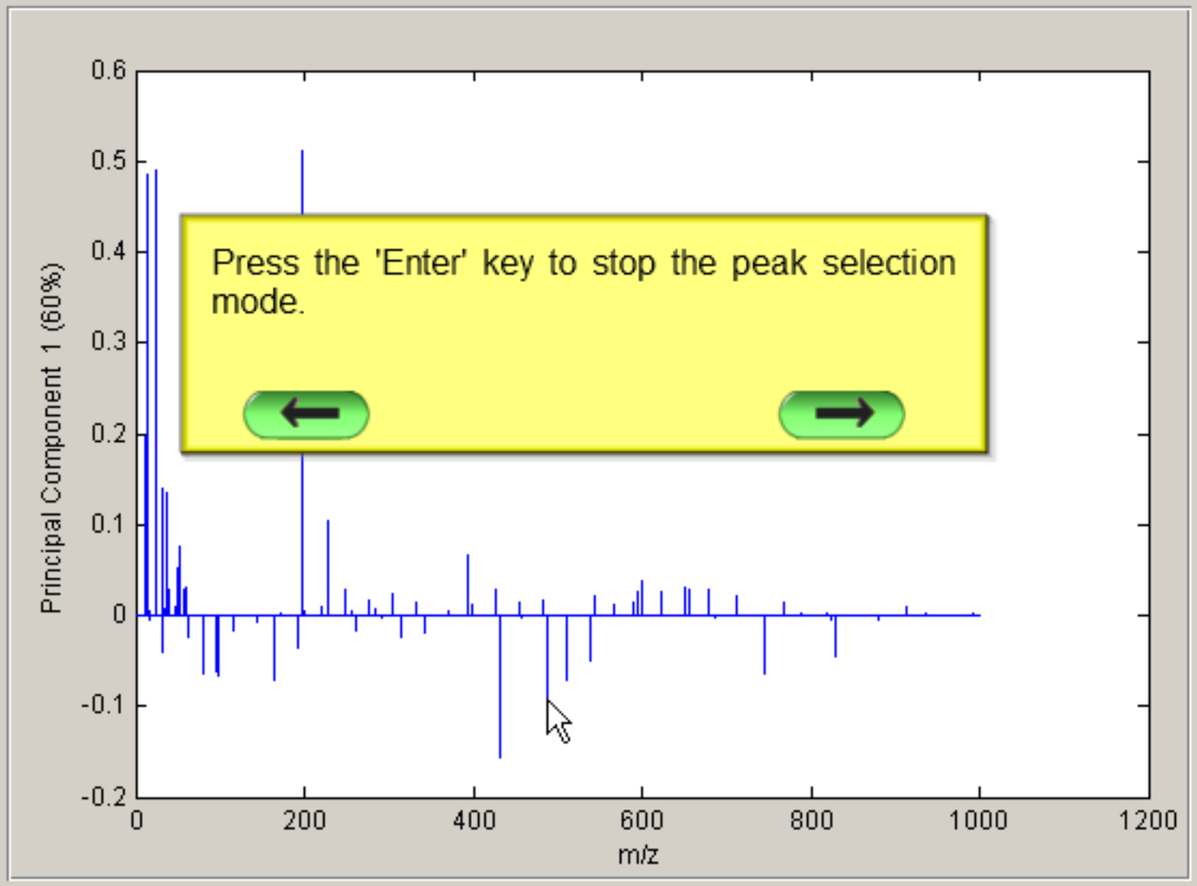
PC# to plot

1

Plot Loads

Save Figure

Close Panel



Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Creat Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

Choose Peaks

Label Custom

Close Panel

spectragui

File Data Pre-Processing MVA Data Display extra

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	samplenames

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
newscores	newloads	newvar	newmodel

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: newloads
Variables: exactmass
% Variance: newvar

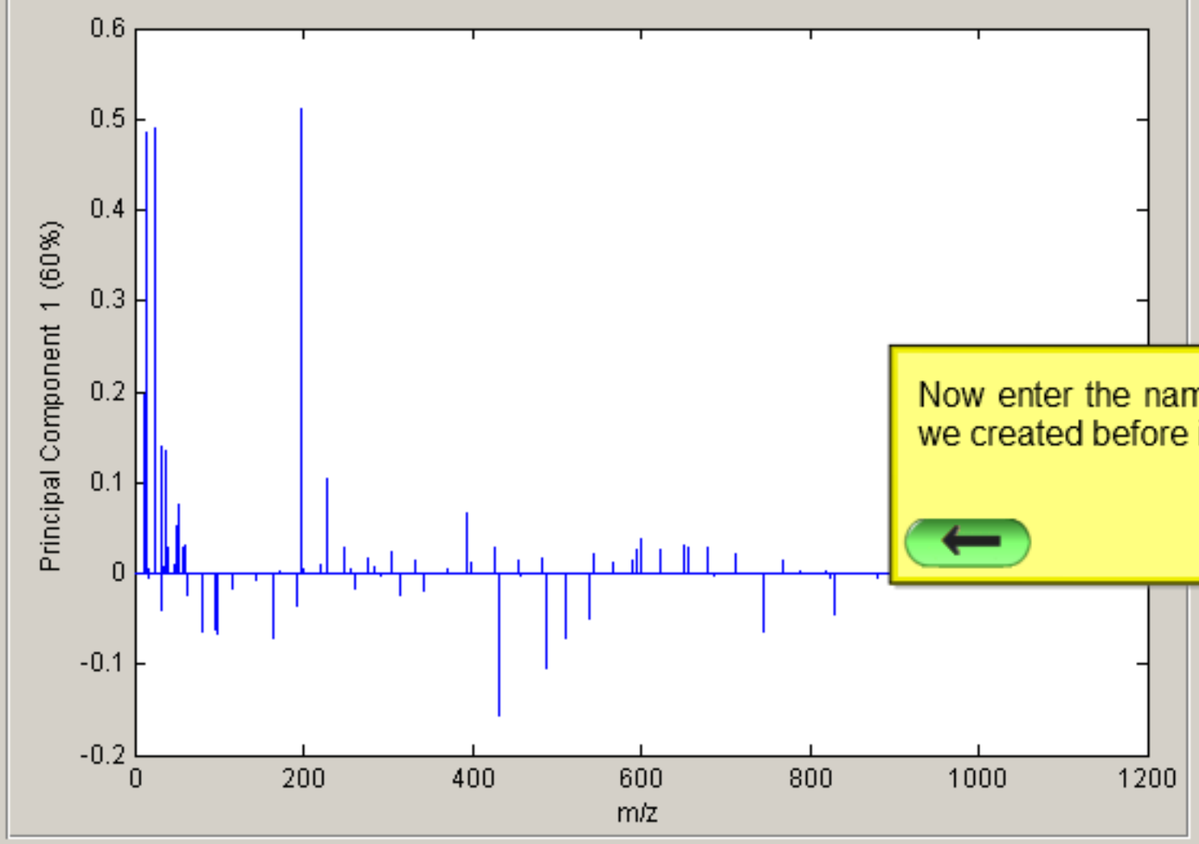
PC# to plot

1

Plot Loads

Save Figure

Close Panel



Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Creat Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

customlabels

Label Custom

Now enter the name of the custom labels we created before in this box.

Close Panel

spectragui

File Data Pre-Processing MVA Data Display extra

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	samplenames

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
newscores	newloads	newvar	newmodel

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: newloads
Variables: exactmass
% Variance: newvar

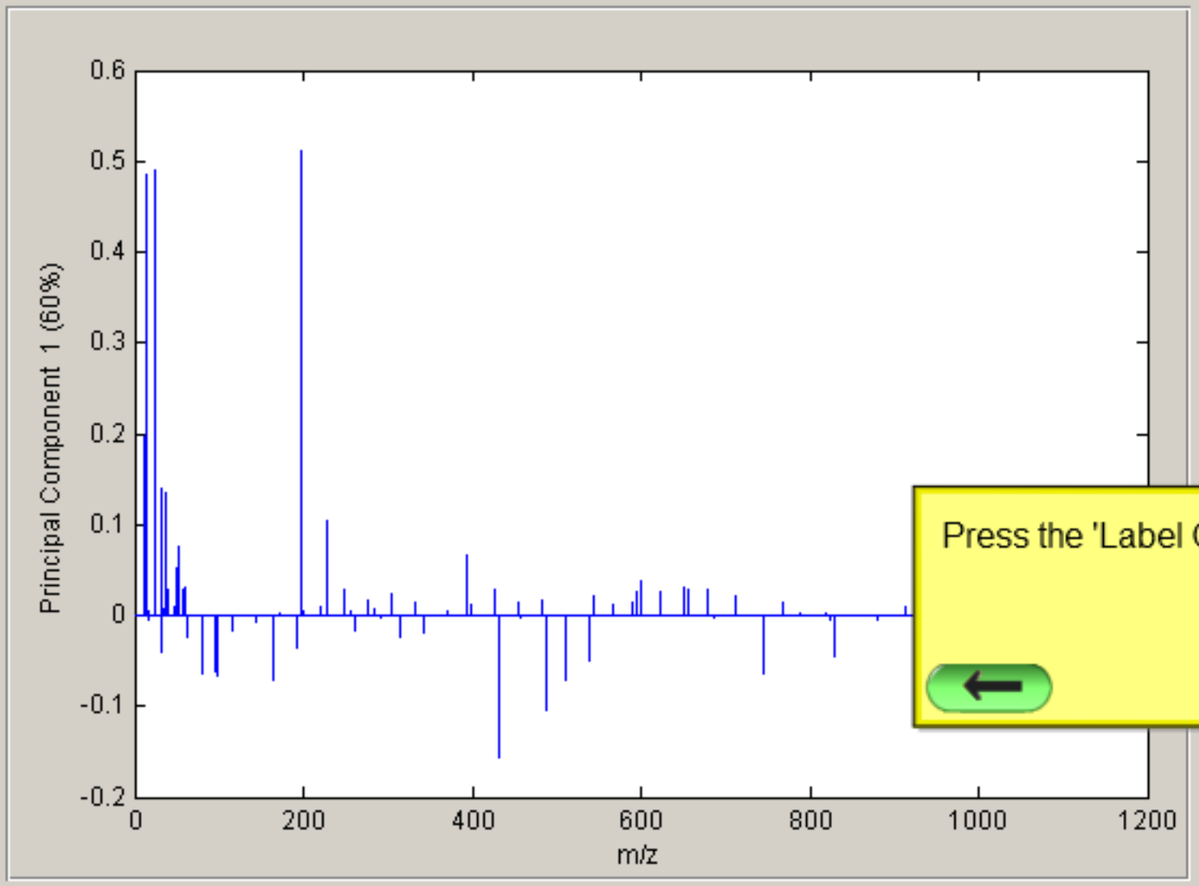
PC# to plot

1

Plot Loads

Save Figure

Close Panel



Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Creat Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

customlabels

Label Custom

Press the 'Label Custom' button.

Close Panel

spectragui

File Data Pre-Processing MVA Data Display extra

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix: ndatass
Name of Variable Matrix: exactmass
Name of Filename Matrix: filenames
Name of Totalcounts Matrix: totalcounts
Name of Samplenames Matrix: samplenames

MVA Data Selection Panel

Name of Scores Matrix: newscores
Name of Loadings Matrix: newloads
Name of % Variance Matrix: newvar
Name of Model Matrix: newmodel

Plot Loadings

Load Selected Data

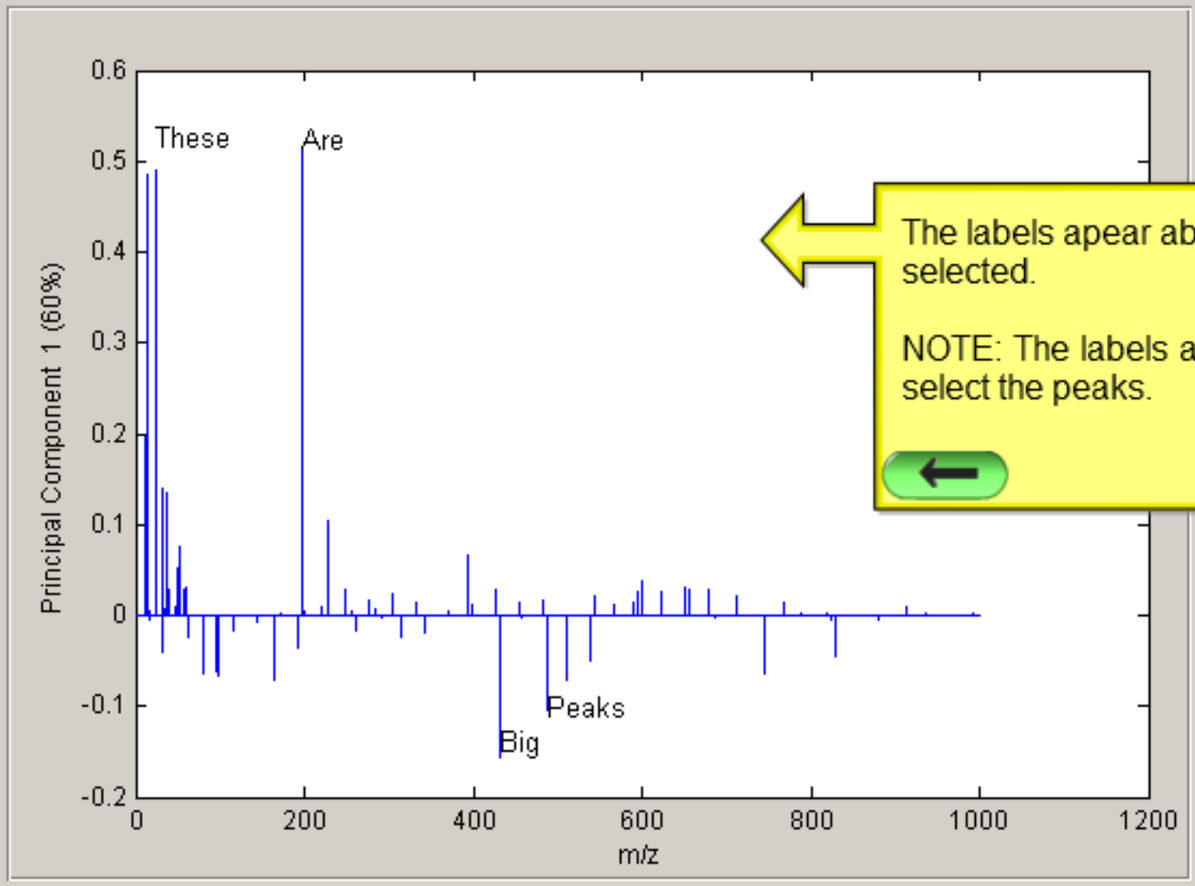
Load Selected Data

Loaded Data

Loadings: newloads
Variables: exactmass
% Variance: newvar

PC# to plot: 1

Plot Loads | Save Figure | Close Panel



The labels apear above the peaks that you selected.

NOTE: The labels appear in the order you select the peaks.

Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Creat Raw Data Plot For Labeled Peaks

custom labels
elected peaks.

Custom Labels to use: customlabels

Choose Peaks

Label Custom

Close Panel

spectragui

File Data Pre-Processing MVA Data Display extra

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	samplenames

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
newscores	newloads	newvar	newmodel

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: newloads
Variables: exactmass
% Variance: newvar

PC# to plot

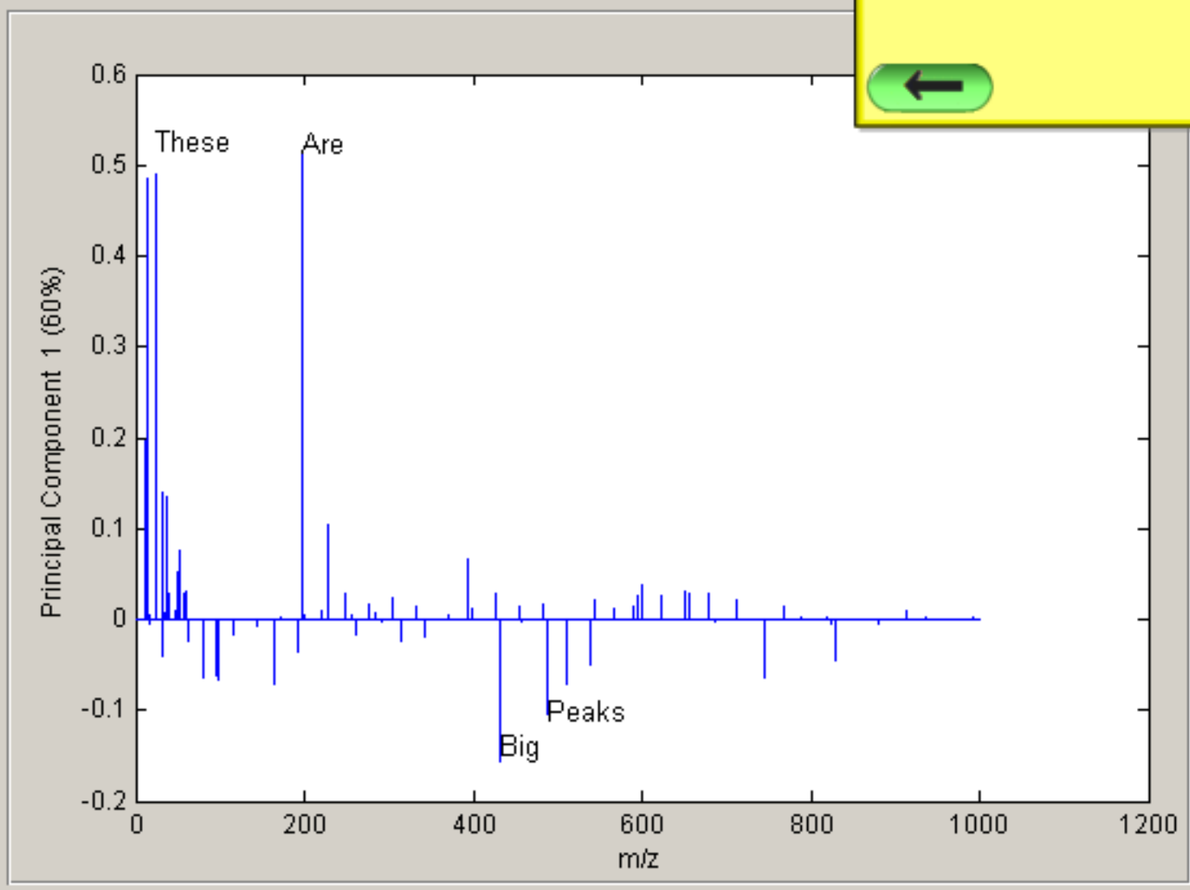
1

Plot Loads

Save Figure

Push this to save the

You can save the figure using the 'Save Figure' button.



Label Loadings

Label all peaks above a threshold value.

Label Peaks

Label Threshold

a Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

customlabels

Choose Peaks

Label Custom

Close Panel

spectragui

Save picture as

Save in: MATLAB

- slices
- asdfdddd.jpg
- ddddddd.jpg
- default.jpg
- defaultssdss.jpg
- Overlay3dSnapShot.jpg
- OverlayXYSnapShot.jpg
- OverlayXZSnapShot.jpg
- OverlayYZSnapShot.jpg
- test1.jpg
- test2.jpg

My Recent Documents · Desktop · My Documents · My Computer · My Network Places

File name: customlabeledplot — Save

Save as type: jpeg (*.jpg) — Cancel

nel

r analysis unless you specify otherwise.
ation you want to use in your analysis.

ix **Name of Totalcounts Matrix**: totalcounts — **Name of Samplenames Matrix**: samplenames

Panel

ix **Name of Model Matrix**: newmodel

Label Loadings

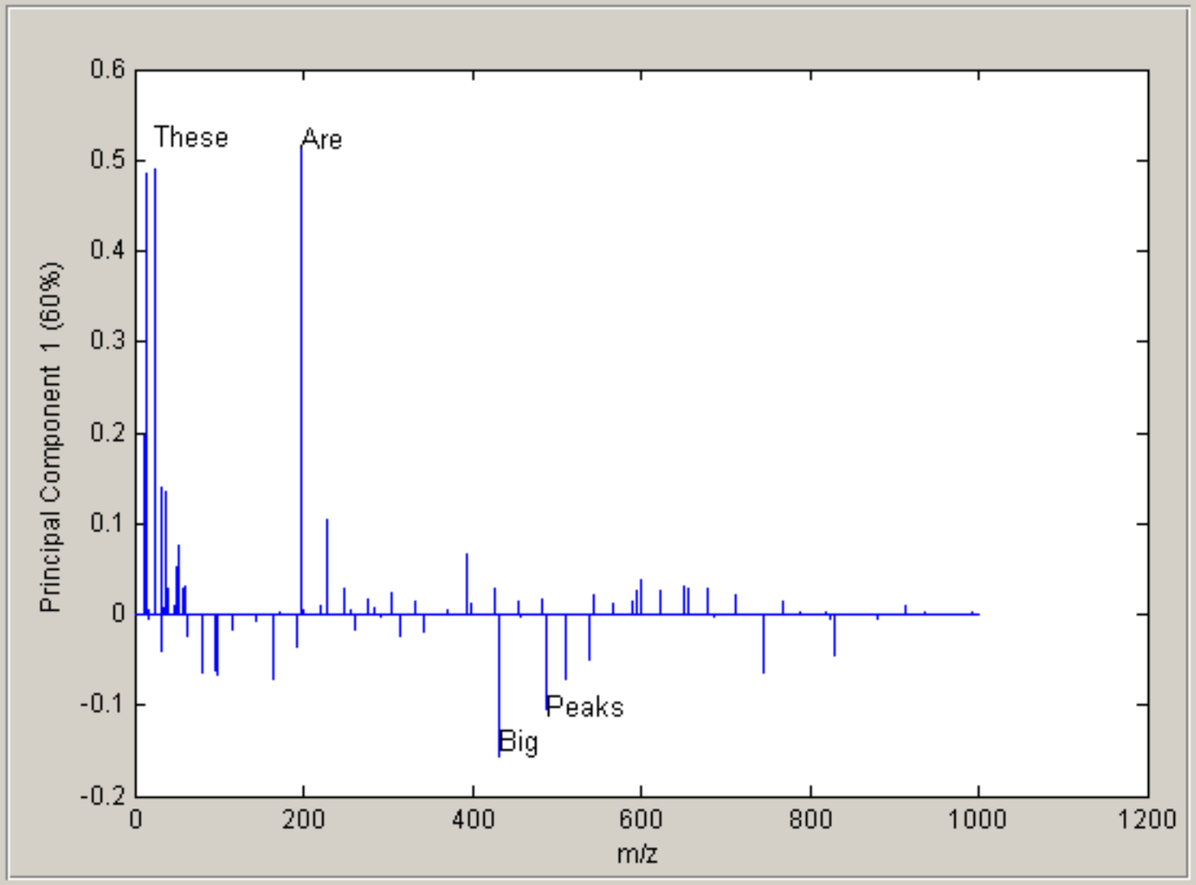
This dialog allows you to save the figure where you want and in the format that you want.

Give the figure a name and press the save button.

Creat Raw Data Plot For Labeled Peaks

PC# to plot 1

Plot Loads | **Save Figure** | **Close Panel**



Use custom labels for selected peaks.

Custom Labels to use: customlabels

Choose Peaks | **Label Custom**

Close Panel

spectragui

File Data Pre-Processing MVA Data Display extra

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	samplenames

MVA Data Selection Panel

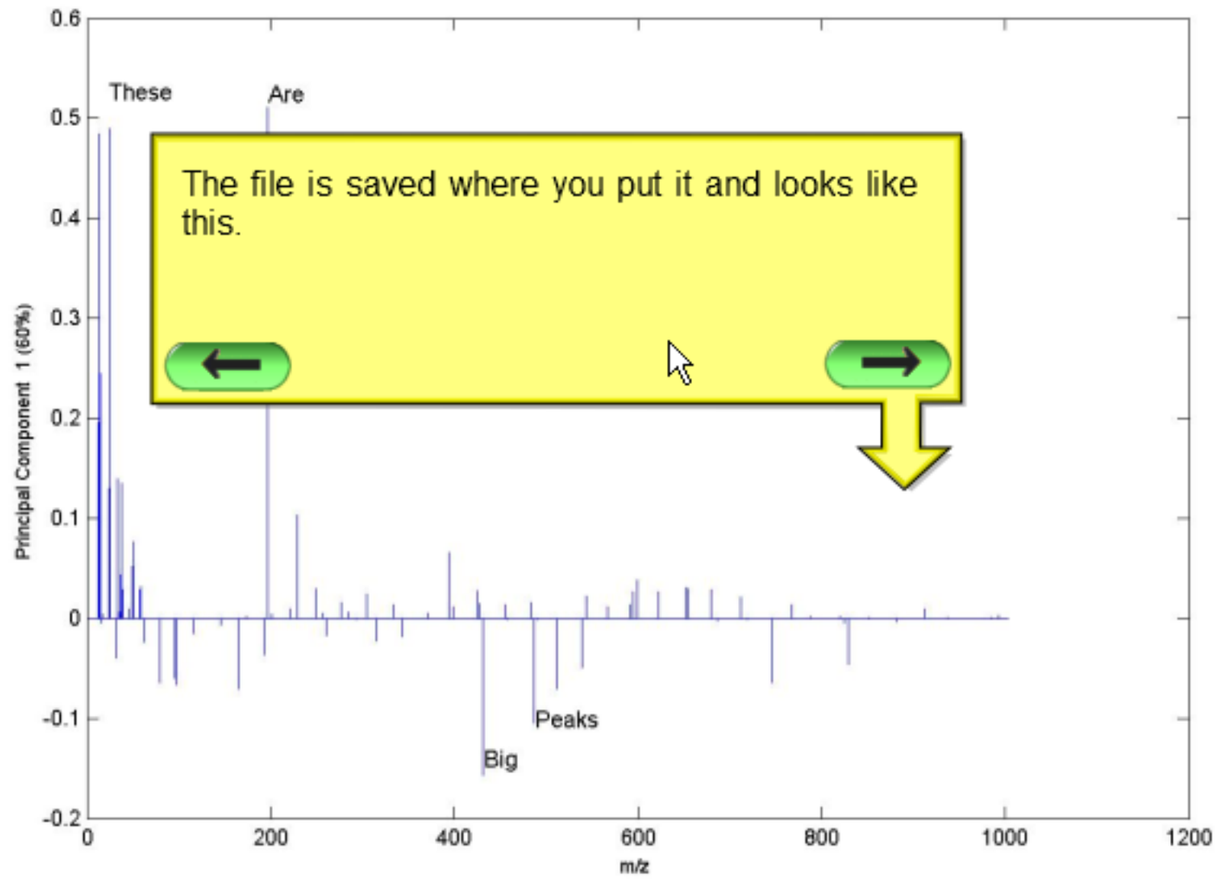
Name of Scores Matri

newscores

customlabeledplot.jpg - IrfanView (Zoom: 595 x 446)

File Edit Image Options View Help

7/26



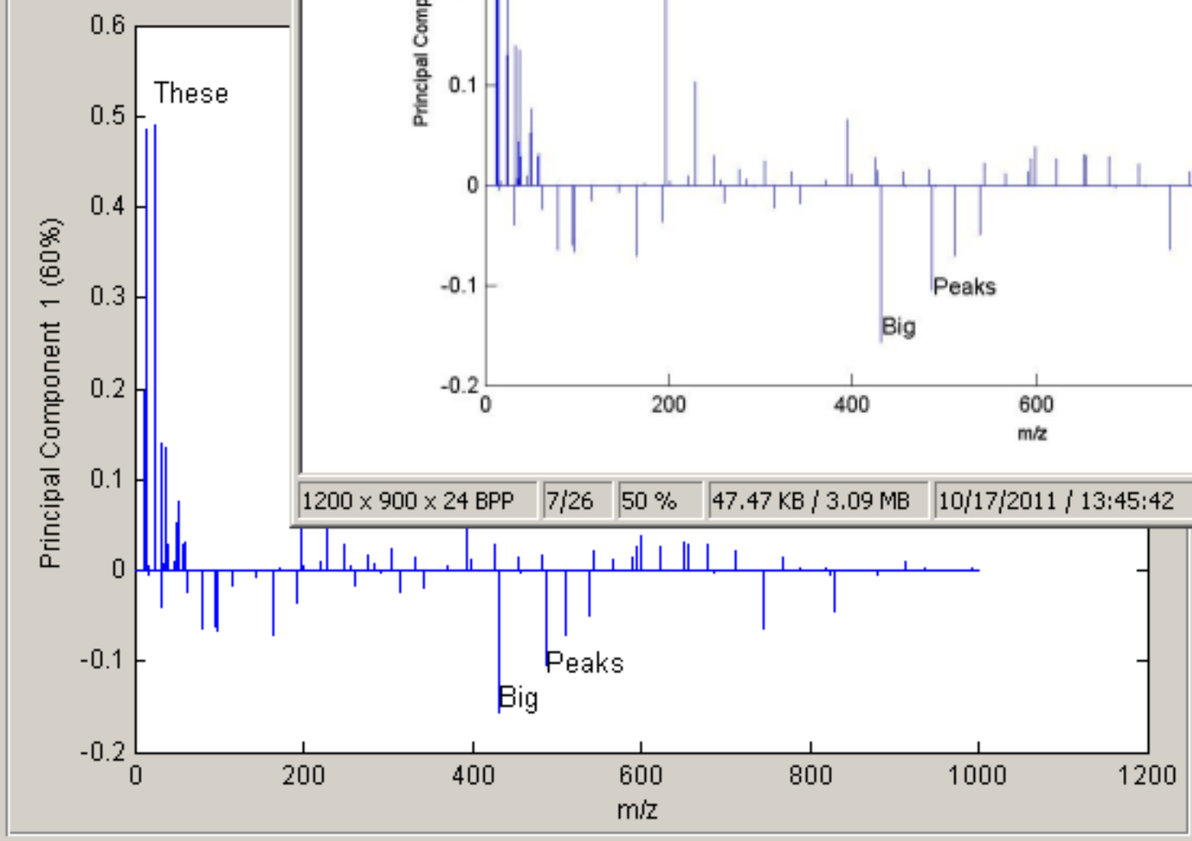
1200 x 900 x 24 BPP | 7/26 | 50 % | 47.47 KB / 3.09 MB | 10/17/2011 / 13:45:42

Load Selected Da

Load Selected Da

PC# to plot

1



ings

l Threshold

Labeled Peaks

n labels
peaks.

Custom Labels
to use

customlabels

Label Custom

Close Panel

spectragui

File Data Pre-Processing MVA Data Display

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatat	exactmass	filenames	totalcounts	samplenames

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
scores	loads	var	model

Plot Loadings

Load Selected Data

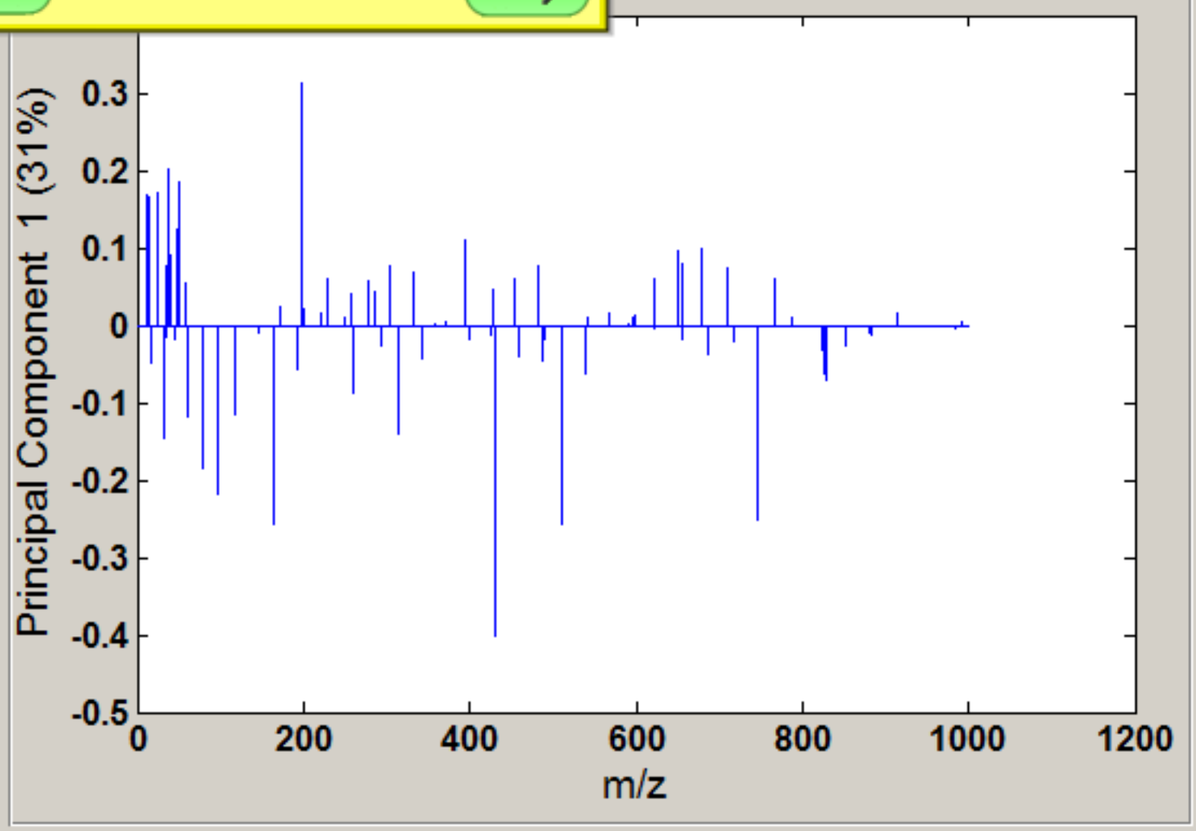
Load Selected Data

Loaded Data

Loadings:	loads
Variables:	exactmass
% Variance:	var

You can make an external figure by pressing the 'Make Ext' button.

Make Ext Close Panel



Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Creat Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

Choose Peaks Label Custom

Close Panel

spectragui

File Data Pre-Processing MVA Data Display

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.

ur analysis.

Name of Data Matr

ndatat

Matrix

Name of Samplenames Matrix

samplenames

Name of Scores Ma

scores

trix

Load Selected I

Load Selected I

Label Loadings

eaks above

old value.

Peaks

ove

Label Threshold

w Data Plot For Labeled Peaks

Use custom labels
for selected peaks.

Custom Labels
to use

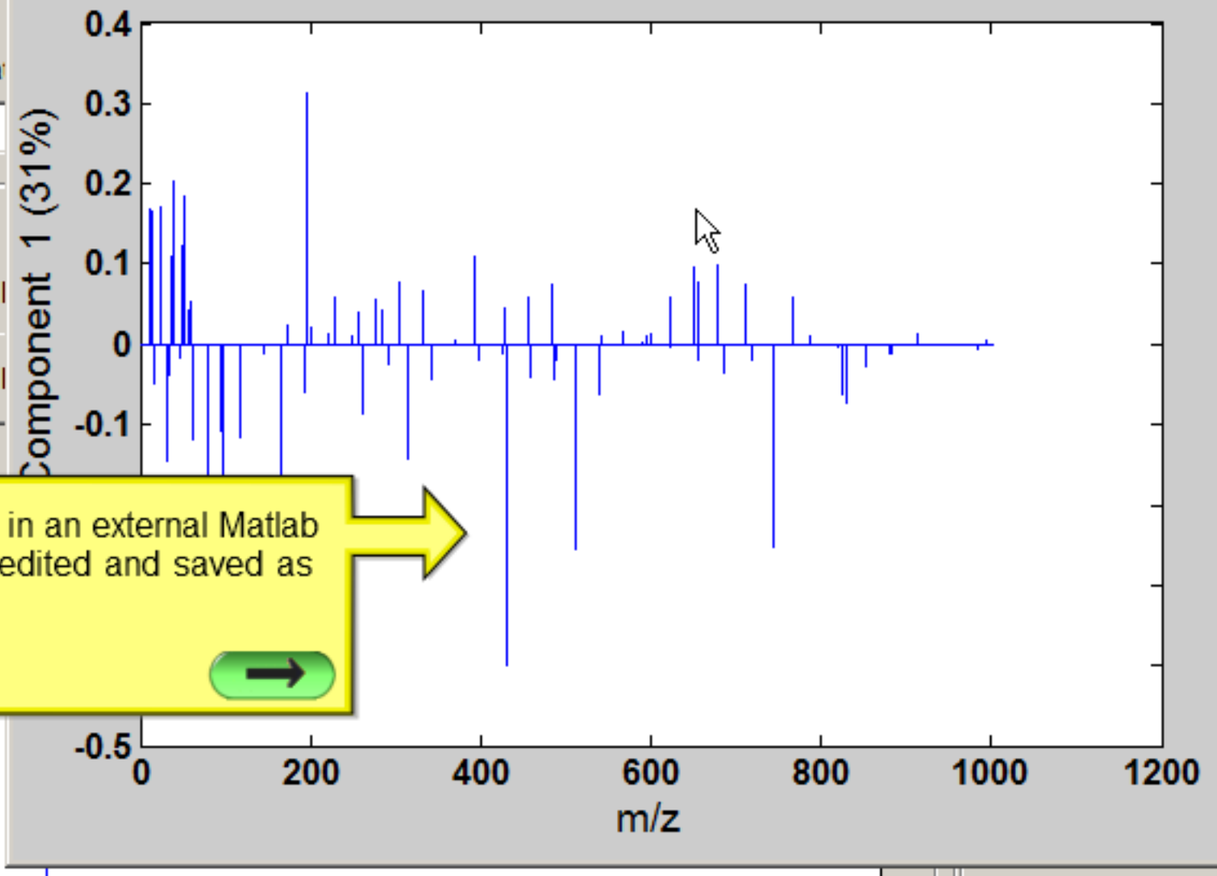
Choose Peaks

Label Custom

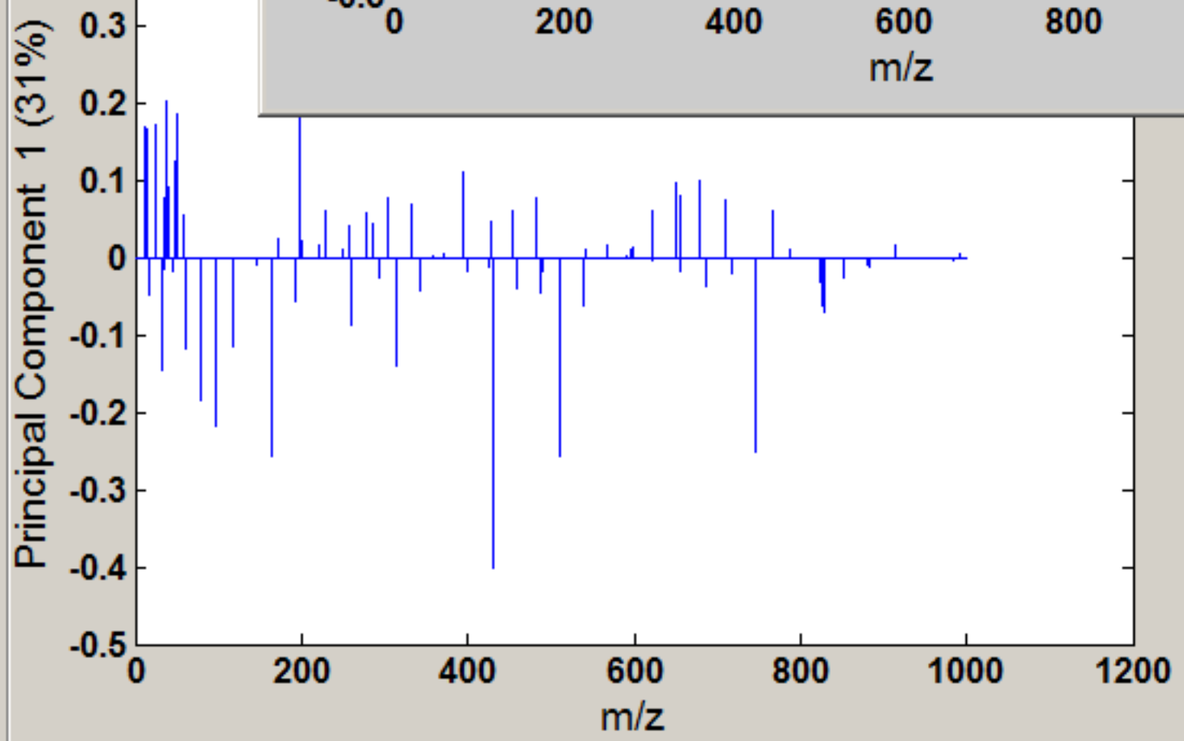
Close Panel

Figure 4

File Edit View Insert Tools Desktop Window Help



The figure is created in an external Matlab window and can be edited and saved as desired.



spectragui

File Data Pre-Processing MVA Data Display extra

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	samplenames

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
newscores	newloads	newvar	newmodel

Now you can close both panels by pressing this 'Close Panel' button.

Load Selected D

Load Selected D

% Variance: newvar

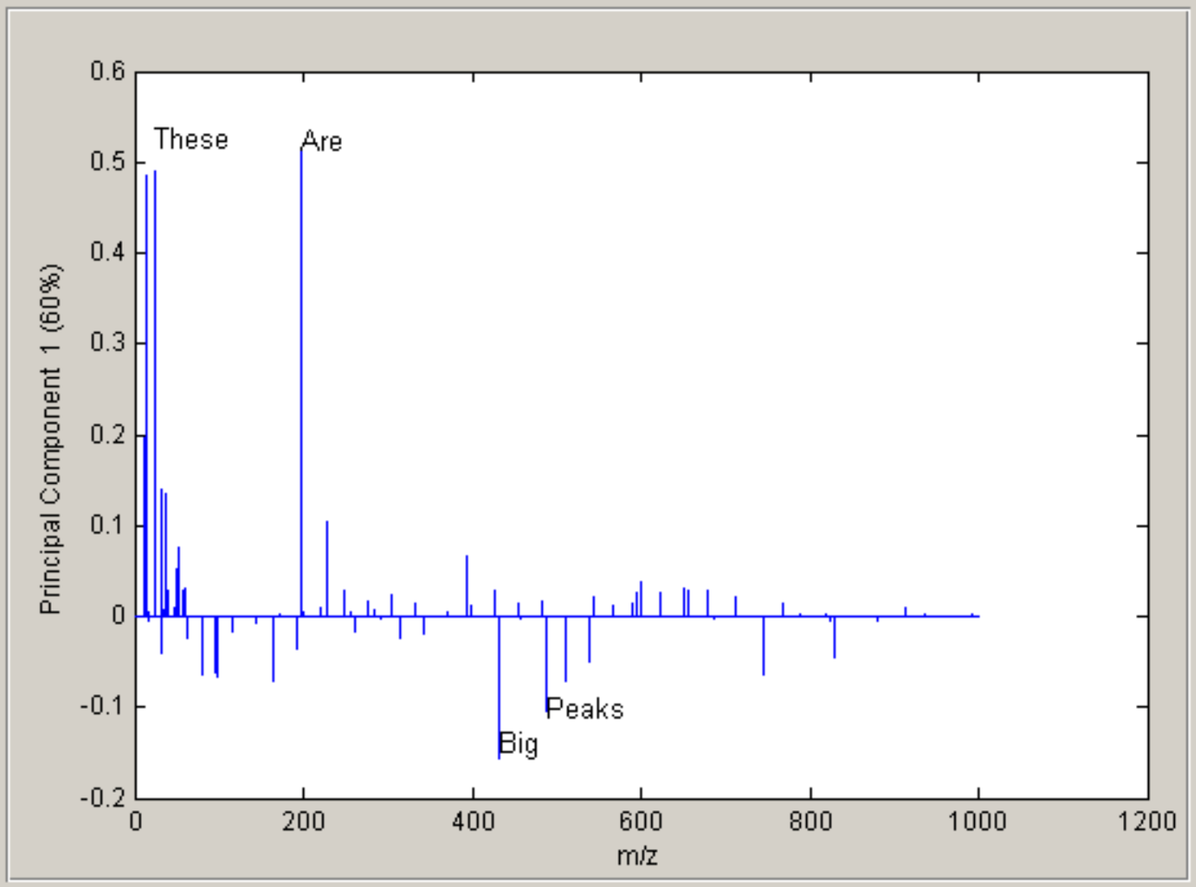
PC# to plot

1

Plot Loads

Save Figure

Close Pane



Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Creat Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

customlabels

Choose Peaks

Label Custom

Close Panel

spectragui

File Data Pre-Processing MVA Data Display extra

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	Select Variables	filenames	totalcounts	samplenames

That's it for this tutorial.

Press the green button on the left to go back to the previous step. Press the button the right to go back to the beginning of the tutorial.