

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

Select Data

Name of Variable Matrix

Select Variables

Name of Filename Matrix

Select Filenames

Name of Totalcounts Matrix

Select Totalcounts

Name of Samplenames Matrix

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.



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

ndatat

Name of Variable Matrix

exactmass

Name of Filename Matrix

filenames

Name of Totalcounts Matrix

totalcounts

Name of Samplenames Matrix

samplenames

This tutorial will cover how to run PCA on your data, create Scores and Loadings plots, Save the plots, and Export the Scores and Loadings data.



- Run PCA
- PCA Modelling
- Run DPCA
- Export MVA Data
- Find Correlated Peaks

To run PCA on the data:
From the 'MVA' menu choose -> 'Run PCA'



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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

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
<input type="text" value="ndatat"/>	<input type="text" value="exactmass"/>	<input type="text" value="filenames"/>	<input type="text" value="totalcounts"/>	<input type="text" value="samplenames"/>

PCA Panel

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

After making sure the correct data is selected above. Press the 'Load Selected Data' button.

← →

Data:	None
Samples:	None
Variables:	None

Scaling Method

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal

Close Panel

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
<input type="text" value="ndatat"/>	<input type="text" value="exactmass"/>	<input type="text" value="filenames"/>	<input type="text" value="totalcounts"/>	<input type="text" value="samplenames"/>

PCA Panel

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: **ndatat**
Samples: **samplenames**
Variables: **exactmass**

Scaling Method

Choose one

- Choose one
- None
- Mean Center
- Autoscale
- SQRT-MeanCenter**

Choose the pre-processing/scaling you want to use from the drop down menu. Here we will choose 'SQRT-MeanCenter'.

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal

Close Panel

Data Selection Panel

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Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
<input type="text" value="ndatat"/>	<input type="text" value="exactmass"/>	<input type="text" value="filenames"/>	<input type="text" value="totalcounts"/>	<input type="text" value="samplenames"/>

PCA Panel

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: **ndatat**
Samples: **samplenames**
Variables: **exactmass**

Scaling Method

Run PCA

Then Press the 'Run PCA' button.

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal

Close Panel

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:

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

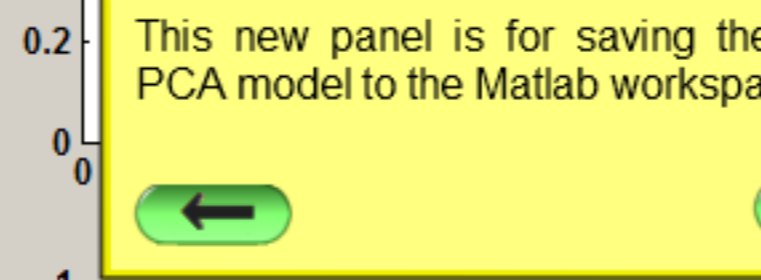
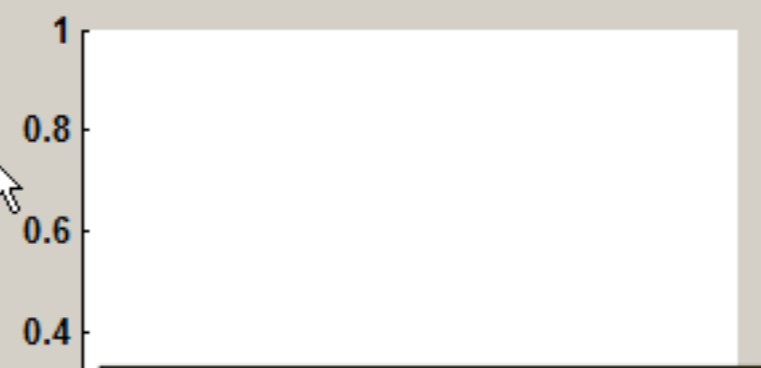
A new panel appears that allows you to quickly browse the scores and loadings plots. These plots can be saved by pressing the 'Ext Plot' button and saving the files as desired.

PCA Panel

Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved. Loading plots default to m/z vs PC#.

X-Axis: Y-Axis:



Save PCA Data to Workspace

Number of PCs to keep

Scores output name

Loadings output name

Percent variance output name

Model output name

Scaling Method

PCA Summary

PC#	%Var	%Vartotal
1	31.4	31.4
2	22.5	53.9
3	18.8	72.7
4	12.3	85
5	8.4	93.4
6	6.1	99.5
7	0.4	99.9
8	0.1	99.9
9	0	99.9
10	0	100

This new panel is for saving the current PCA model to the Matlab workspace.

Data Selection Panel

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Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: **ndatat**
 Samples: **samplenames**
 Variables: **exactmass**

Scaling Method

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	31.4	31.4
2	22.5	53.9
3	18.8	72.7
4	12.3	85
5	8.4	93.4
6	6.1	99.5
7	0.4	99.9
8	0.1	99.9
9	0	99.9
10	0	100

A summary of the PCA model is provided here showing the % variance captured for each PC (%Var) and the cumulative %variance for each sequential PC (%Vartotal).

PCA Panel

Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved.

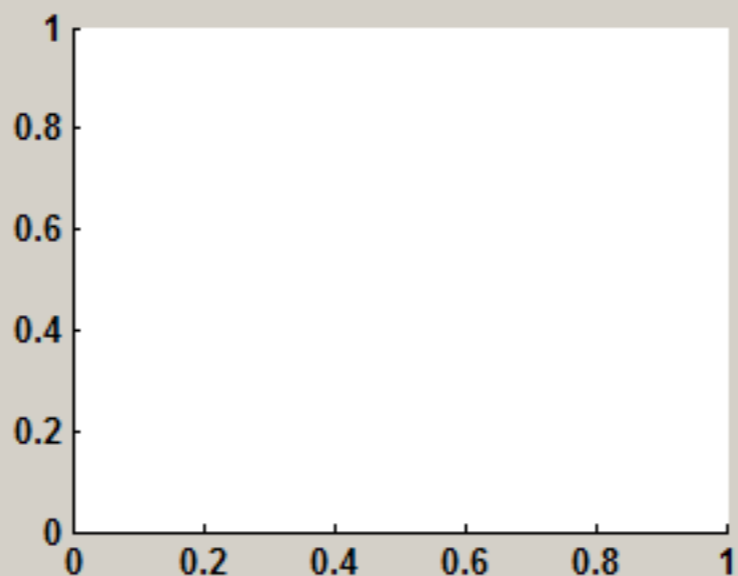
Loading plots default to m/z vs PC#.

X-Axis

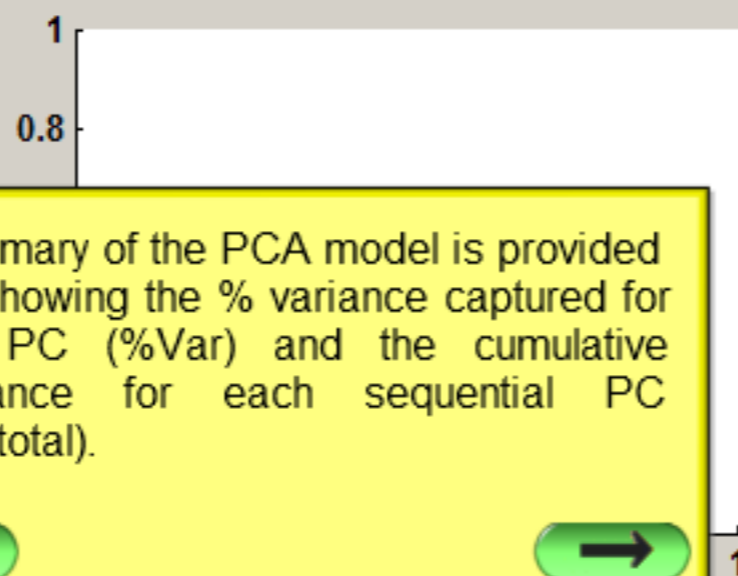
Y-Axis

Plot Scores

Plot Loads



EXT Plot



EXT Plot

Save PCA Data to Workspace

Number of PCs to keep

Scores output name

Loadings output name

Percent variance output name

Model output name

Save To Workspace

Close Panel

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:

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: **ndatat**
 Samples: **samplenames**
 Variables: **exactmass**

Scaling Method

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	31.4	31.4
2	22.5	53.9
3	18.8	72.7
4	12.3	85
5	8.4	93.4
6	6.1	99.5
7	0.4	99.9
8	0.1	99.9
9	0	99.9
10	0	100

PCA Panel

Plot PCA Scores and Loadings

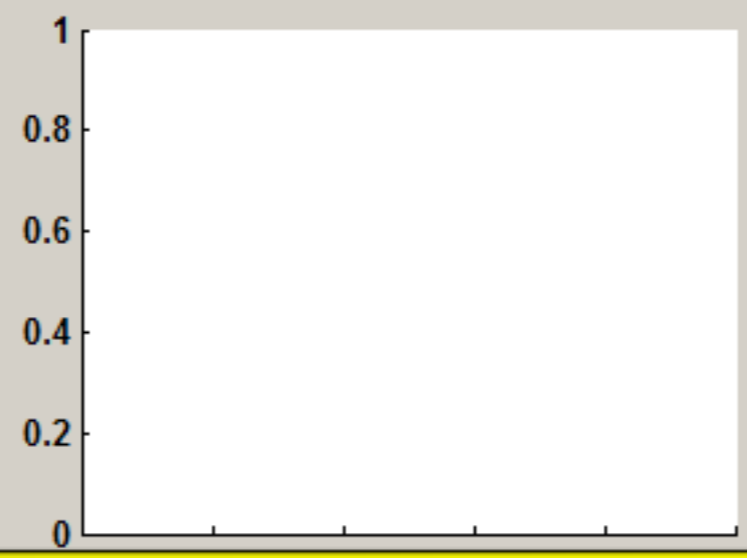
These plots are for a quick check of the results and cannot be saved. Loading plots default to m/z vs PC#.

X-Axis

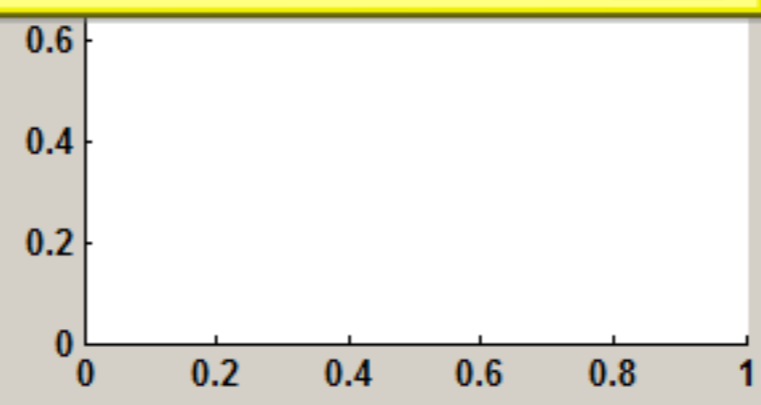
Y-Axis

Plot Scores

Plot Loads



EXT Plot



EXT Plot

Save PCA Data to Workspace

Number of PCs to keep

Scores output name

Loadings output name

Percent variance output name

Model output name

Save To Workspace

Close Panel

Press the 'Show Eigenvalue Scree Plot' to see a plot of the eigenvalue vs PC number.

← →

Data Selection Panel

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Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: **ndatat**
 Samples: **samplenames**
 Variables: **exactmass**

Scaling Method

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

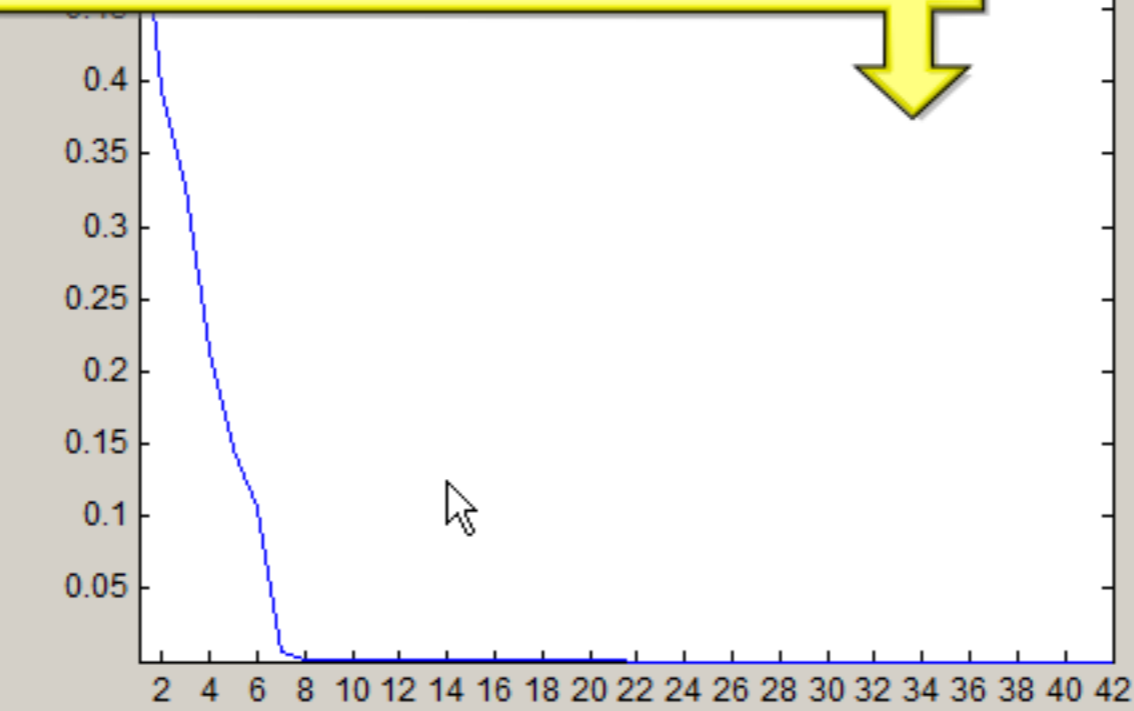
PC#	%Var	%Vartotal
1	31.4	31.4
2	22.5	53.9
3	18.8	72.7
4	12.3	85
5	8.4	93.4
6	6.1	99.5
7	0.4	99.9
8	0.1	99.9
9	0	99.9
10	0	100

PCA Panel

This is a plot of the eigenvalue vs PC number. This plot is often used to decide how many PCs to keep in a model.

The "rule of thumb" is to look for an inflection point in the line and keep the PCs before that inflection point.

In this data set it looks like there is an inflection point at PC 6 or 8.



Close

Save PCA Data to Workspace

Number of PCs to keep

Scores output name

Loadings output name

Percent variance output name

Model output name

Save To Workspace

Close Panel

Data Selection Panel

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Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: **ndatat**
 Samples: **samplenames**
 Variables: **exactmass**

Scaling Method

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Var
1	31.4	
2	22.5	
3	18.8	
4	12.3	
5	8.4	99.9
6	6.1	99.9
7	0.4	99.9
8	0.1	99.9
9	0	99.9
10	0	100

PCA Panel

Save PCA Data to Workspace

Number of PCs to keep

Scores output name

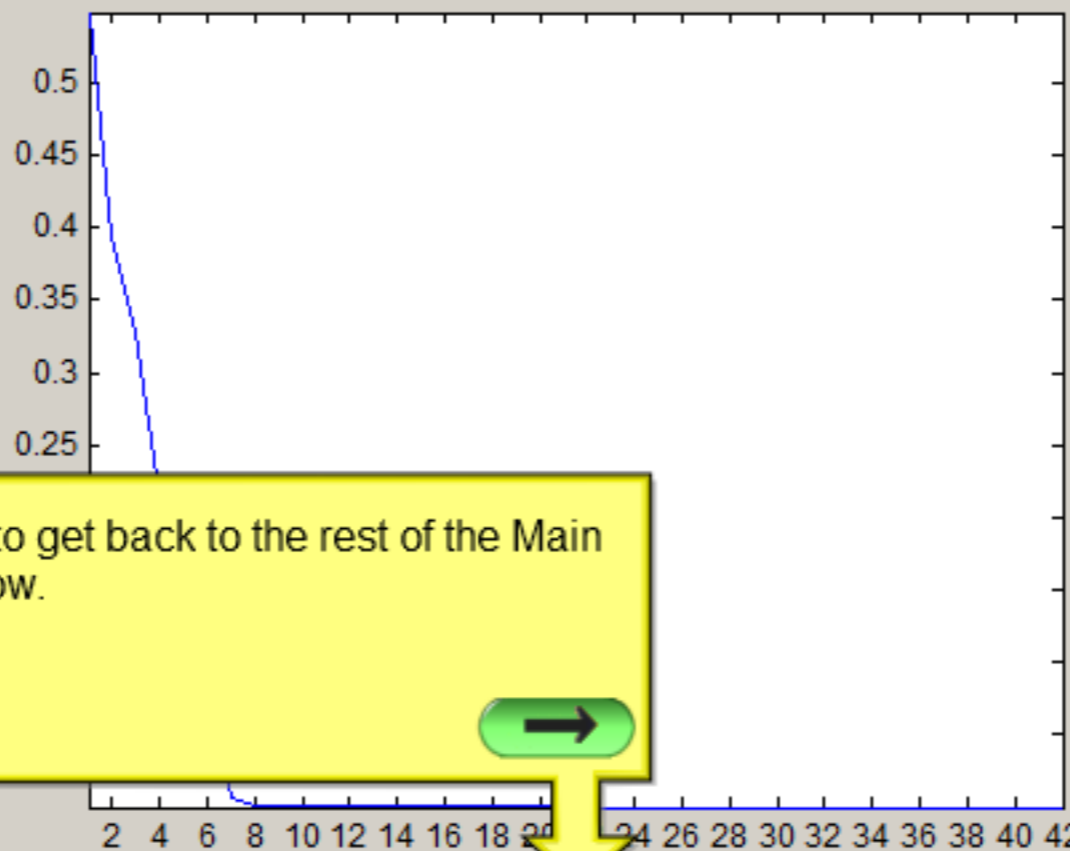
Loadings output name

Percent variance output name

Model output name

Save To Workspace

Eigenvalue Scree Plot



Close this panel to get back to the rest of the Main PCA panel window.

← →

Close

Close Panel

Data Selection Panel

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Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

PCA Panel

Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved.

Loading plots default to m/z vs PC#.

X-Axis

Y-Axis

PC#
PC#
samp/var
1

PC#

Plot Loads

To create a plot, choose which axes you want to plot from the drop down menus.

Scores and loadings plots are most easily interpreted when plotting 1 PC at a time.

Here we will use the sample number for the x axis.

Save PCA Data to Workspace

Number of PCs to keep

Scores output name

Loadings output name

Percent variance output name

Model output name

Save To Workspace

Close Panel

Data:
Samples:
Variables:

Scaling

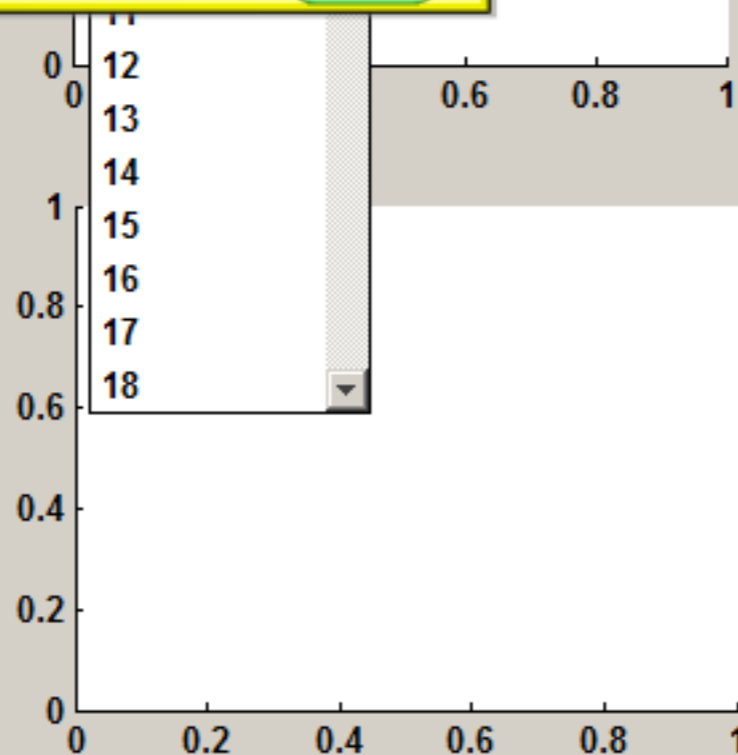
SQRT-Me

Run

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	31.4	31.4
2	22.5	53.9
3	18.8	72.7
4	12.3	85
5	8.4	93.4
6	6.1	99.5
7	0.4	99.9
8	0.1	99.9
9	0	99.9
10	0	100



EXT Plot

EXT Plot

Data Selection Panel

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Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data:
Samples:
Variables:

Scaling

SQRT-Me



Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	31.4	31.4
2	22.5	53.9
3	18.8	72.7
4	12.3	85
5	8.4	93.4
6	6.1	99.5
7	0.4	99.9
8	0.1	99.9
9	0	99.9
10	0	100

PCA Panel

Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved.

Loading plots default to m/z vs PC#.

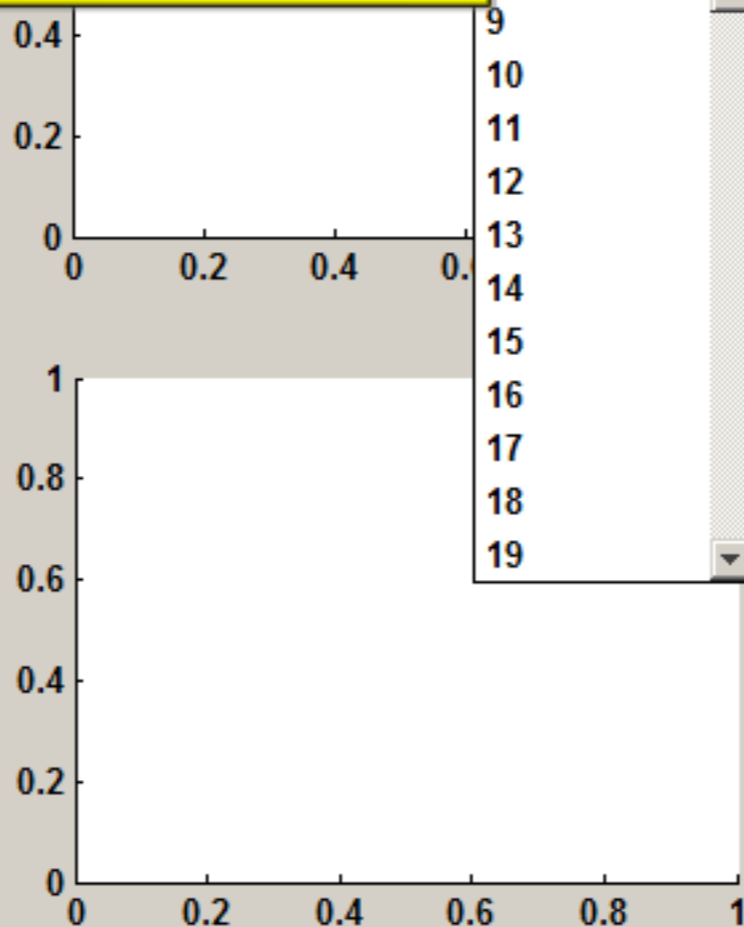
X-Axis

Y-Axis

Plot Scores

And plot PC1 on the y axis.

- PC#
- 1
- 2
- 3
- 4
- 5
- 6
- 7
- 8
- 9
- 10
- 11
- 12
- 13
- 14
- 15
- 16
- 17
- 18
- 19



EXT Plot

EXT Plot

Save PCA Data to Workspace

Number of PCs to keep

Scores output name

Loadings output name

Percent variance output name

Model output name

Save To Workspace

Close Panel

Data Selection Panel

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Name of Data Matrix:
 Name of Variable Matrix:
 Name of Filename Matrix:
 Name of Totalcounts Matrix:
 Name of Samplenames Matrix:

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: **ndatat**
 Samples: **samplenames**
 Variables: **exactmass**

Scaling Method

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	31.4	31.4
2	22.5	53.9
3	18.8	72.7
4	12.3	85
5	8.4	93.4
6	6.1	99.5
7	0.4	99.9
8	0.1	99.9
9	0	99.9
10	0	100

PCA Panel

Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved.

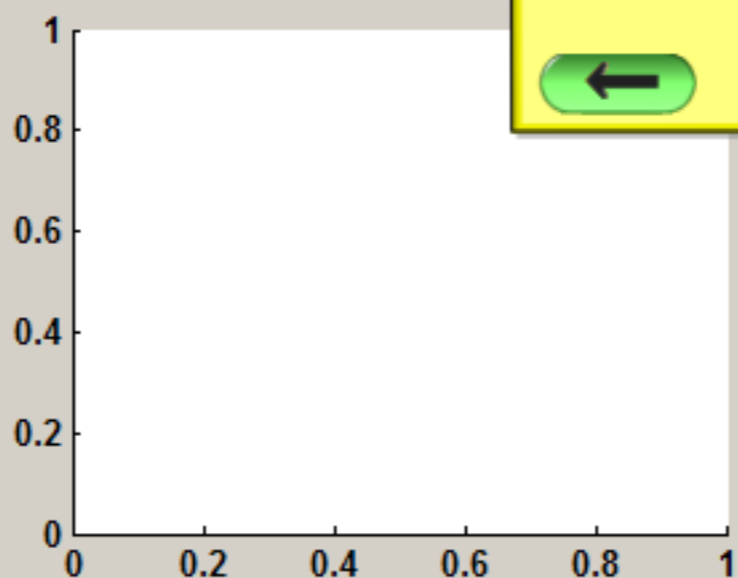
Loading plots default to m/z vs PC#.

X-Axis

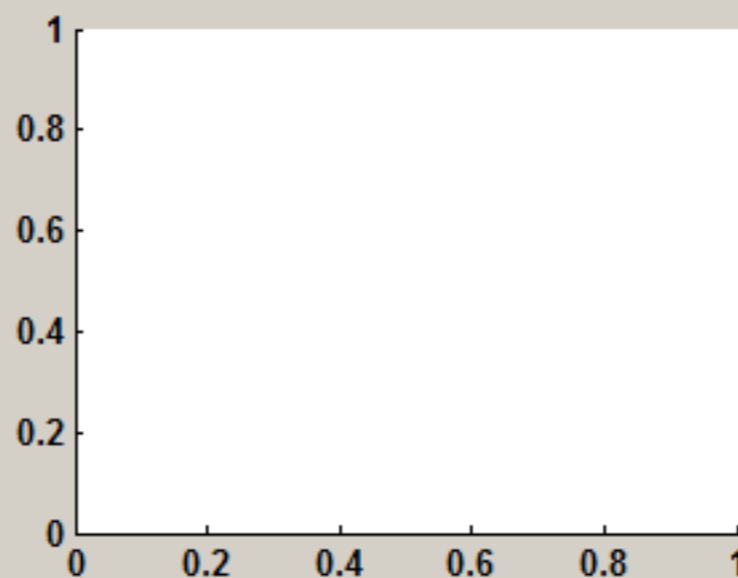
Y-Axis

Plot Scores

Press the 'Plot Scores' button to see a scores plot.



EXT Plot



EXT Plot

Save PCA Data to Workspace

Number of PCs to keep

Output name

Output name

Percent variance output name

Model output name

Save To Workspace

Close Panel

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.

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Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: **ndatat**
 Samples: **samplenames**
 Variables: **exactmass**

Scaling Method

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	31.4	31.4
2	22.5	53.9
3	18.8	72.7
4	12.3	85
5	8.4	93.4
6	6.1	99.5
7	0.4	99.9
8	0.1	99.9
9	0	99.9
10	0	100

PCA Panel

Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved.

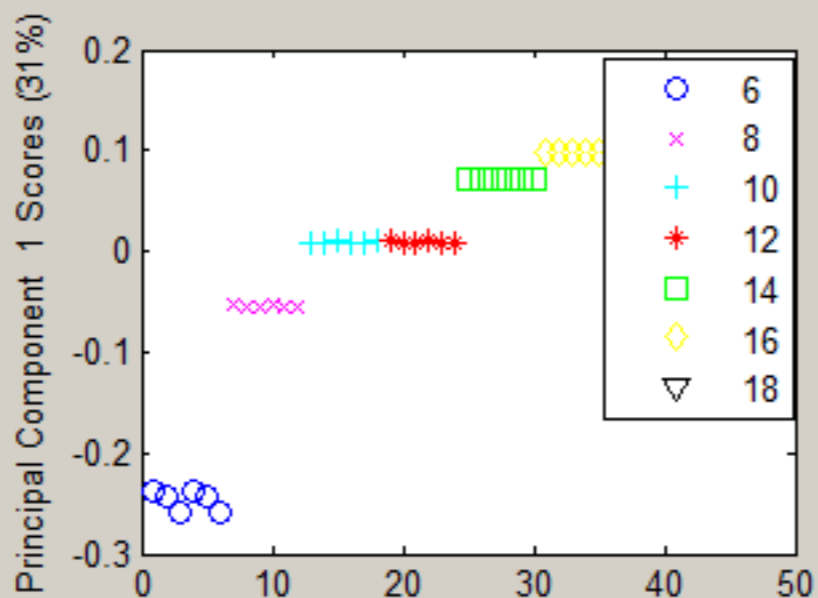
Loading plots default to m/z vs PC#.

X-Axis

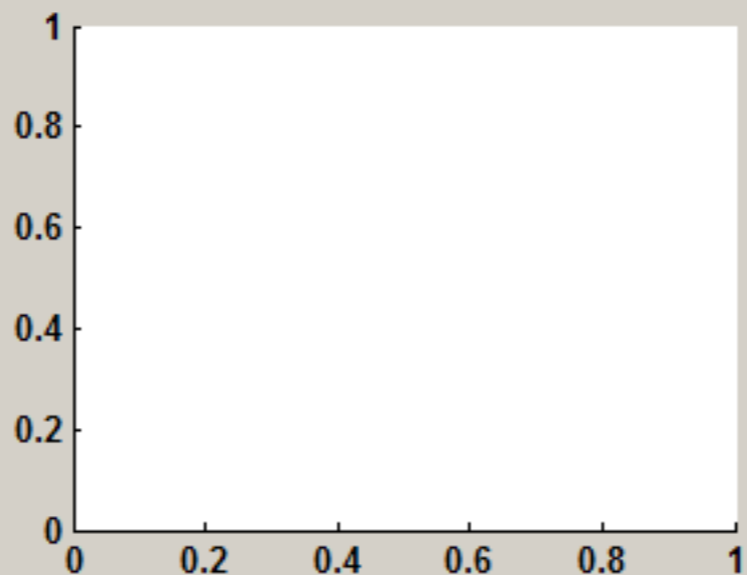
Y-Axis

Plot Scores

Plot Loads



EXT Plot



EXT Plot

Save PCA Data to Workspace

Number of PCs to keep

Scores output name

Press the 'Plot Loads' button to see a Loadings plot.



Percent variance output name

Model output name

Save To Workspace

Close Panel

Data Selection Panel

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Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

PCA Panel

Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved.

Loading plots default to m/z vs PC#.

X-Axis: Y-Axis:

The scores plot is shown here.

← Load Selected Data Plot Loads →

Data: **ndatat**
 Samples: **samplenames**
 Variables: **exactmass**

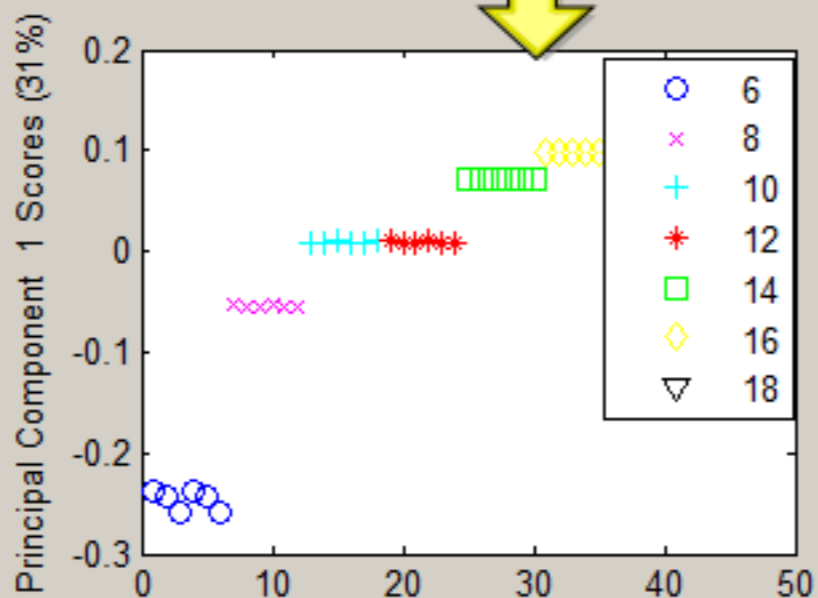
Scaling Method

Run PCA

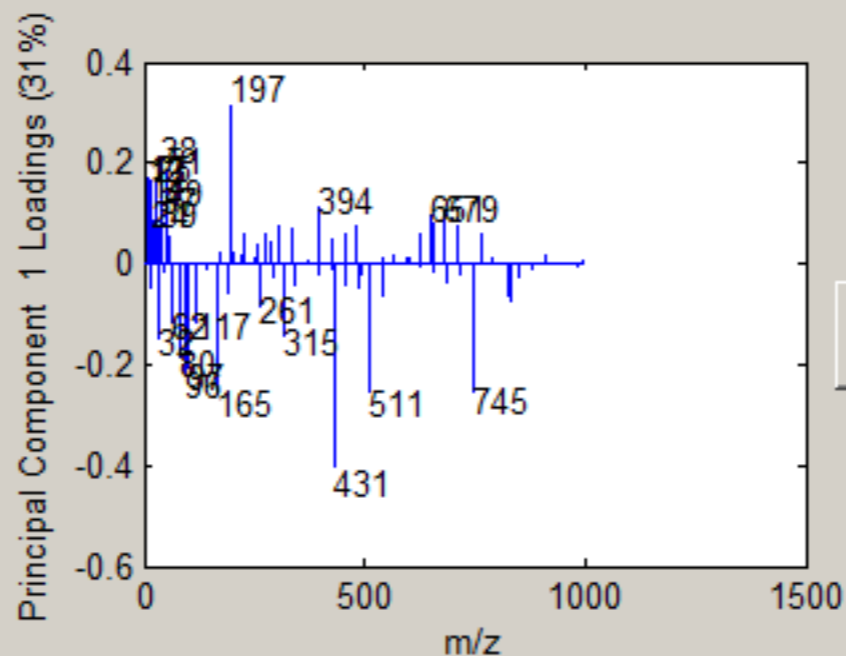
Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	31.4	31.4
2	22.5	53.9
3	18.8	72.7
4	12.3	85
5	8.4	93.4
6	6.1	99.5
7	0.4	99.9
8	0.1	99.9
9	0	99.9
10	0	100



EXT Plot



EXT Plot

Save PCA Data to Workspace

Number of PCs to keep

Scores output name

Loadings output name

Percent variance output name

Model output name

Save To Workspace

Close Panel

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.

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Load Selected Data

Data: **ndatat**
 Samples: **samplenames**
 Variables: **exactmass**

Scaling Method

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	31.4	31.4
2	22.5	53.9
3	18.8	72.7
4	12.3	85
5	8.4	93.4
6	6.1	99.5
7	0.4	99.9
8	0.1	99.9
9	0	99.9
10	0	100

PCA Panel

Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved.

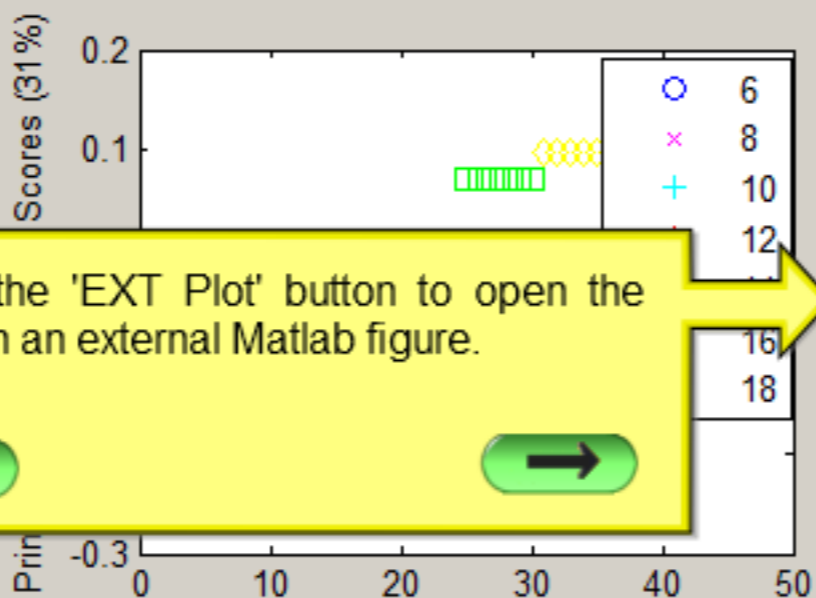
Loading plots default to m/z vs PC#.

X-Axis

Y-Axis

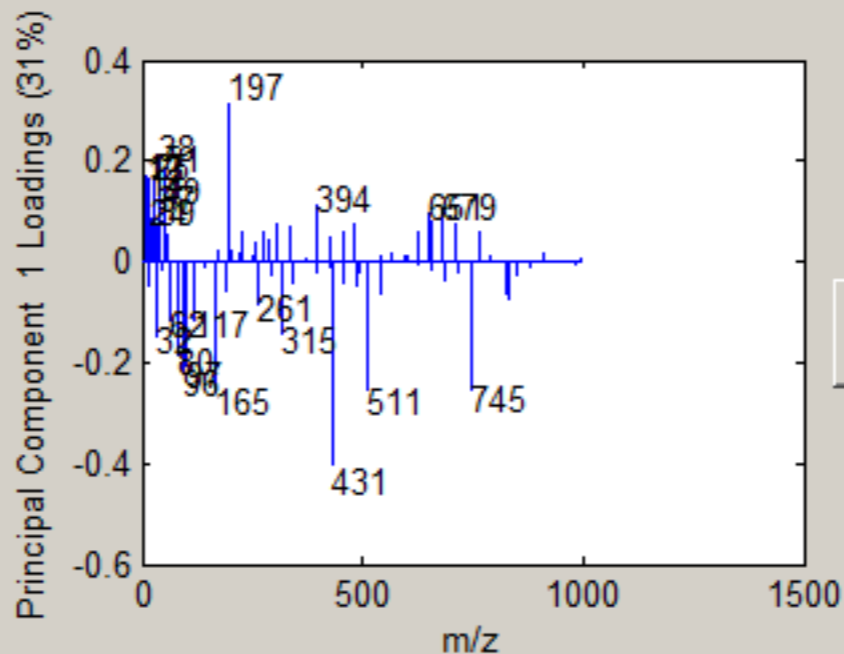
Plot Scores

Plot Loads



EXT Plot

Press the 'EXT Plot' button to open the figure in an external Matlab figure.



EXT Plot

Save PCA Data to Workspace

Number of PCs to keep

Scores output name

Loadings output name

Percent variance output name

Model output name

Save To Workspace

Close Panel

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.

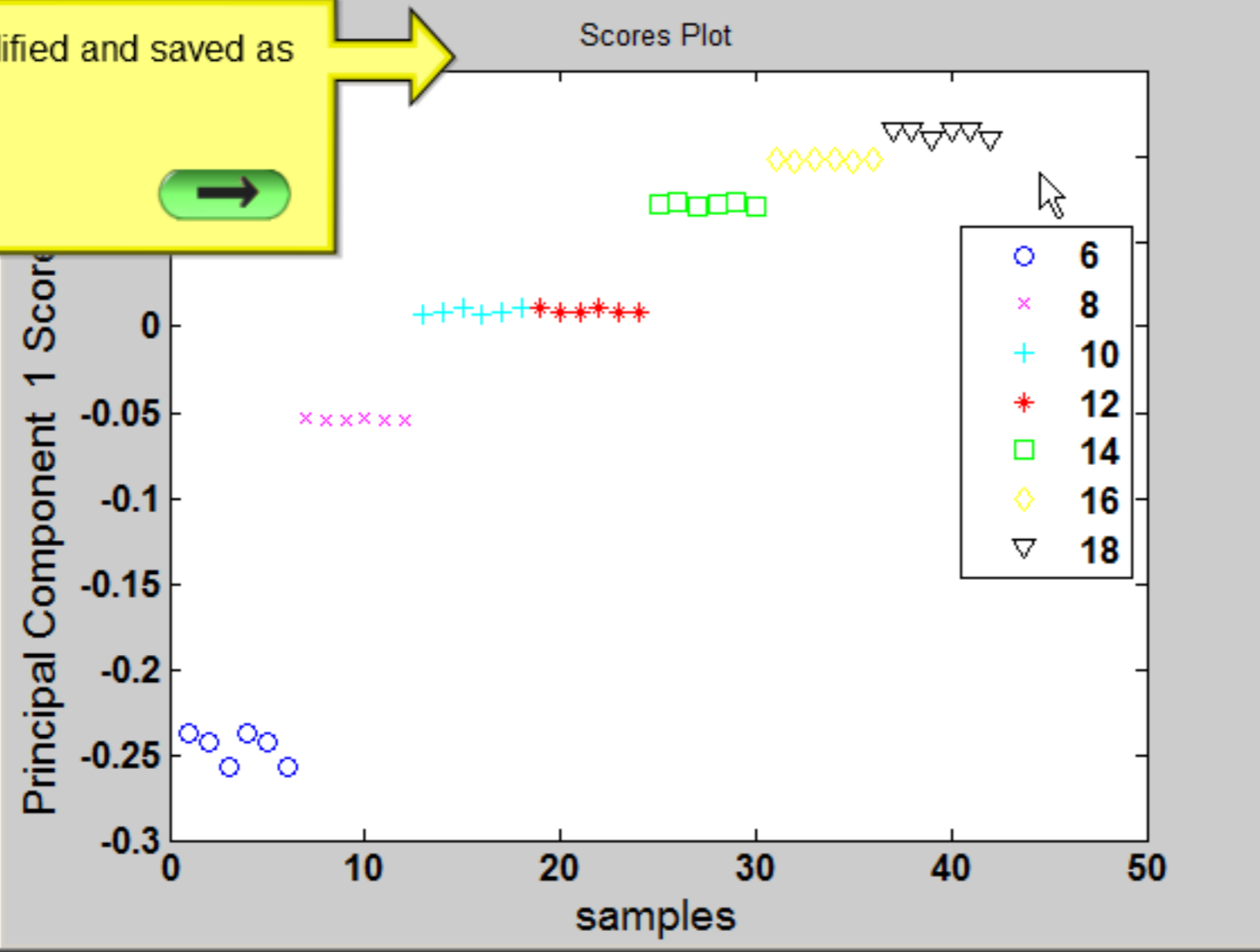
Name of Data Matrix

Name of Samplenames Matrix

Figure 2
 File Edit View Insert Tools Desktop Window Help

This figure can be modified and saved as desired.

← →



Save PCA Data to Workspace

Number of PCs to keep

Scores output name

Loadings output name

Percent variance output name

Model output name

Save To Workspace

Load Selected D

Data: **nda**

Samples: **sample**

Variables: **exactn**

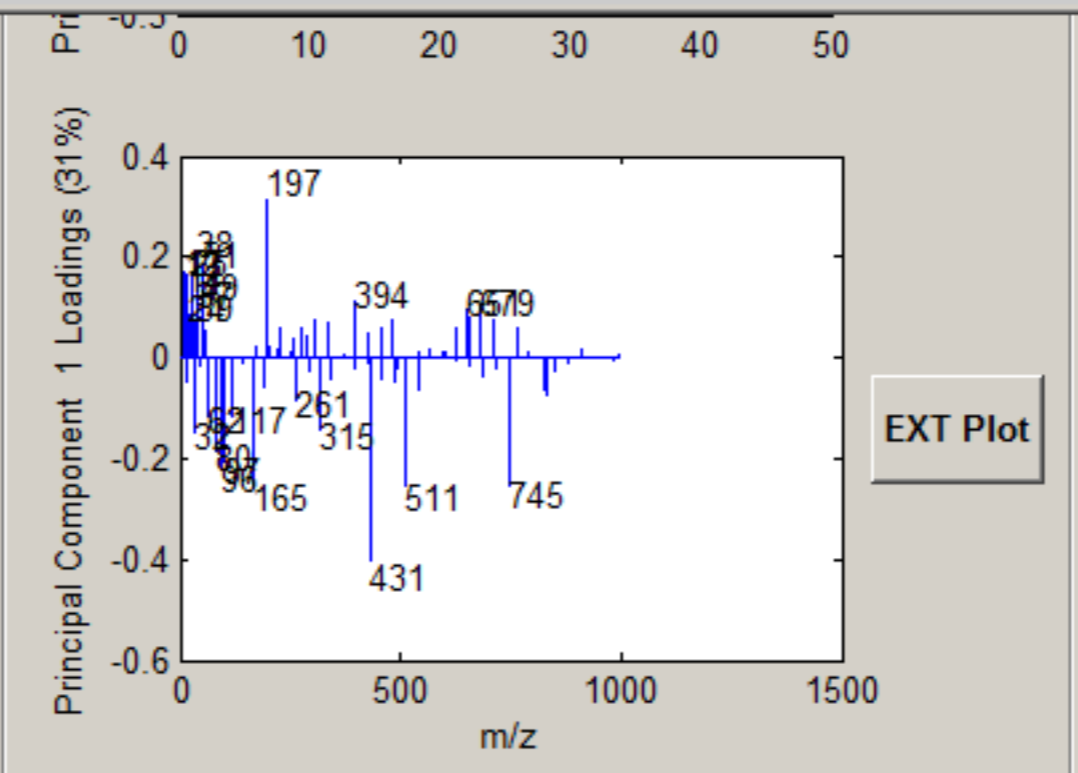
Scaling Metho

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	31.4	31.4
2	22.5	53.9
3	18.8	72.7
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6	6.1	99.5
7	0.4	99.9
8	0.1	99.9
9	0	99.9
10	0	100



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Data Selection Panel

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Input Information

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Load Selected Data

Data: **ndatat**
 Samples: **samplenames**
 Variables: **exactmass**

Scaling Method

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	31.4	31.4
2	22.5	53.9
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4	12.3	85
5	8.4	93.4
6	6.1	99.5
7	0.4	99.9
8	0.1	99.9
9	0	99.9
10	0	100

PCA Panel

Plot PCA Scores and Loadings

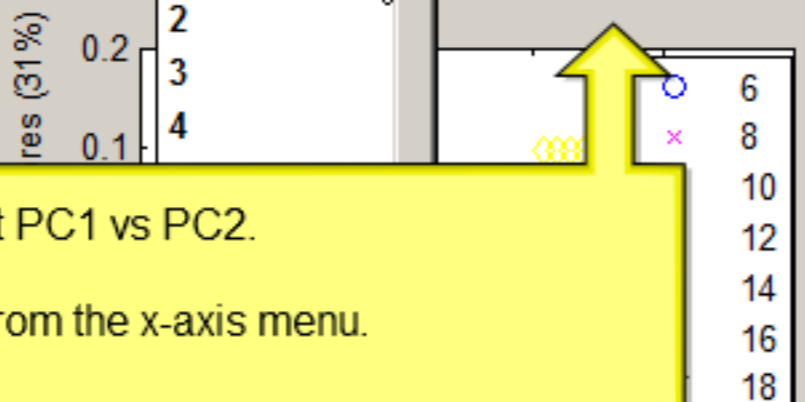
These plots are for a quick check of the results and cannot be saved.

Loading plots default to m/z vs PC#.

X-Axis

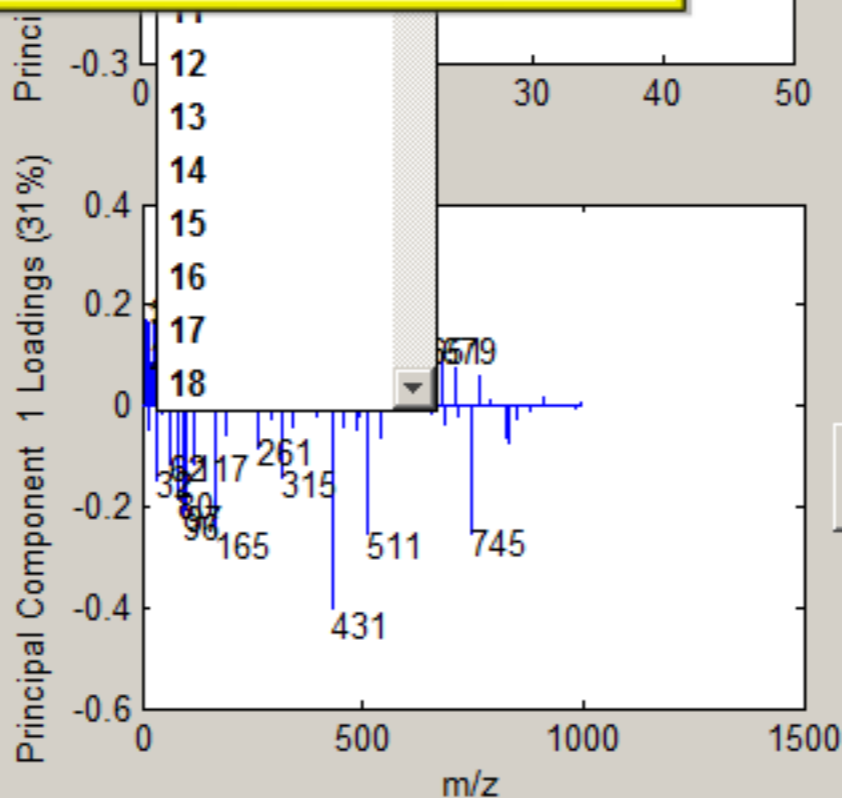
Y-Axis

Plot Loads



EXT Plot

Next we'll plot PC1 vs PC2.
 Select PC1 from the x-axis menu.



EXT Plot

Save PCA Data to Workspace

Number of PCs to keep

Scores output name

Loadings output name

Percent variance output name

Model output name

Save To Workspace

Close Panel

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:

Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load Selected Data

Data: **ndatat**
 Samples: **samplenames**
 Variables: **exactmass**

Scaling Method

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	31.4	31.4
2	22.5	53.9
3	18.8	72.7
4	12.3	85
5	8.4	93.4
6	6.1	99.5
7	0.4	99.9
8	0.1	99.9
9	0	99.9
10	0	100

PCA Panel

Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved.

Loading plots default to m/z vs PC#.

X-Axis

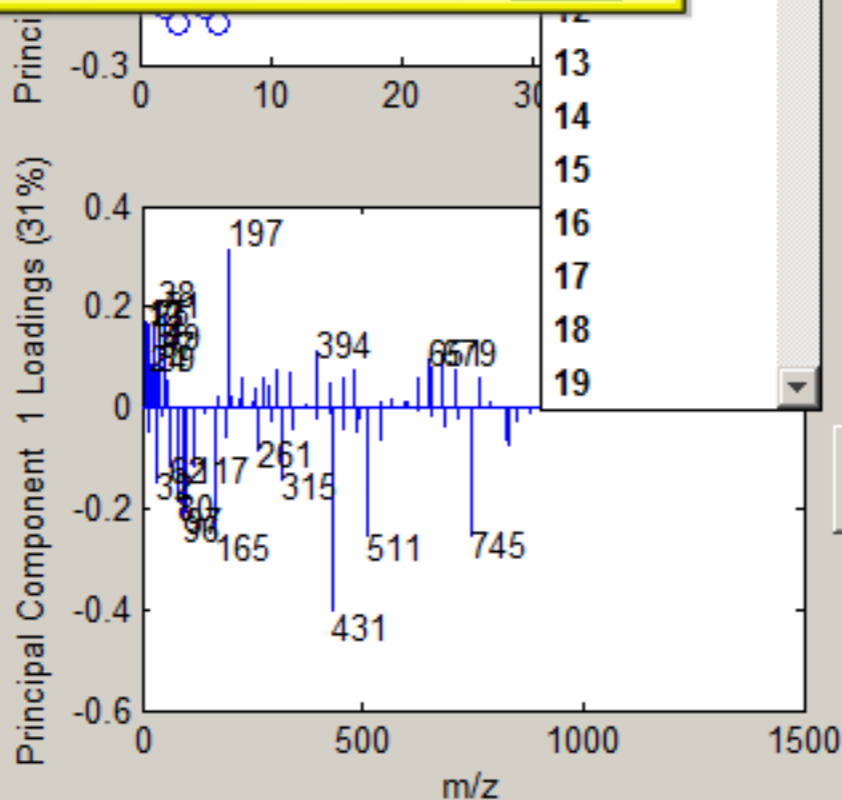
Y-Axis

Plot Scores



And PC2 from the y-axis menu.

EXT Plot



EXT Plot

Save PCA Data to Workspace

Number of PCs to keep

Scores output name

Loadings output name

Percent variance output name

Model output name

Save To Workspace

Close Panel

Data Selection Panel

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Input Information

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Press the 'Plot Scores' button to update the scores plot.

← →

PCA Panel

Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved.

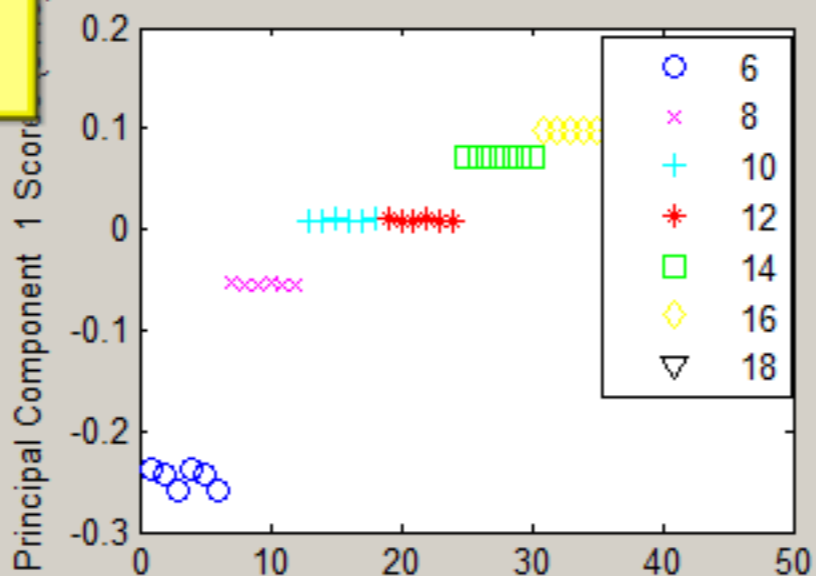
Loading plots default to m/z vs PC#.

X-Axis

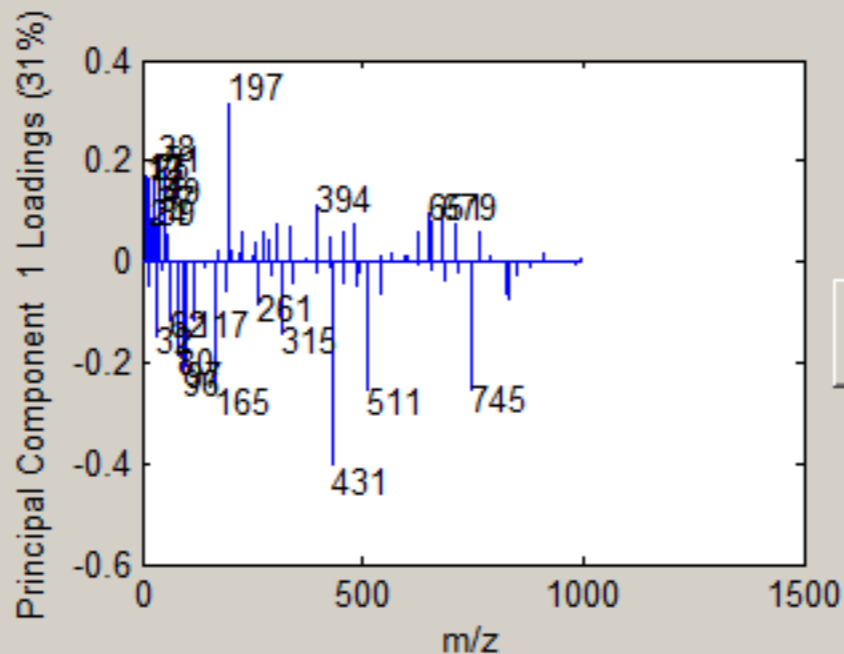
Y-Axis

Plot Scores

Plot Loads



EXT Plot



EXT Plot

Save PCA Data to Workspace

Number of PCs to keep

Scores output name

Loadings output name

Percent variance output name

Model output name

Save To Workspace

Close Panel

Scaling Method

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

PC#	%Var	%Vartotal
1	31.4	31.4
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4	12.3	85
5	8.4	93.4
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Input Information

Make sure the data selected above is the data you want to analyze and then press the "Load Selected Data" button.

Load S

Data:
Samples:
Variables:

Scaling Method

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

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9	0	99.9
10	0	100

PCA Panel

Plot PCA Scores and Loadings

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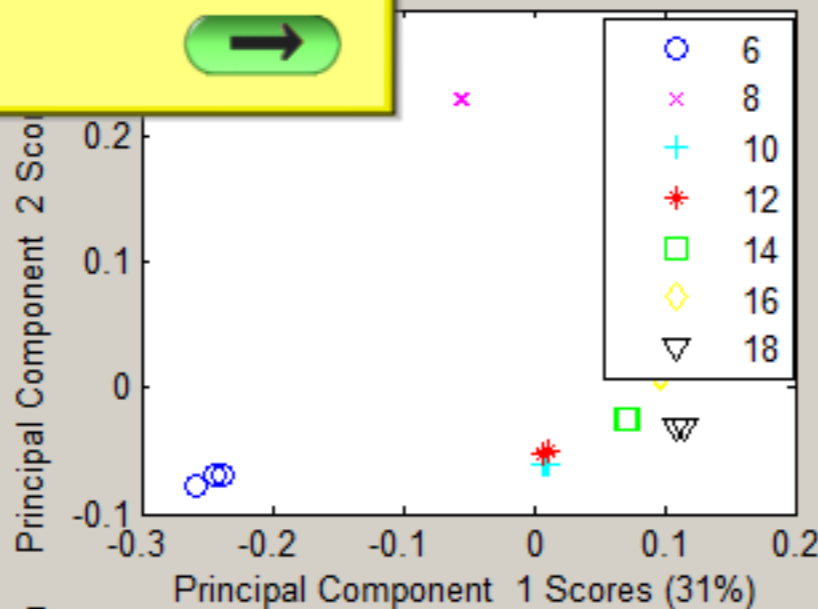
Loading plots default to m/z vs PC#.

X-Axis

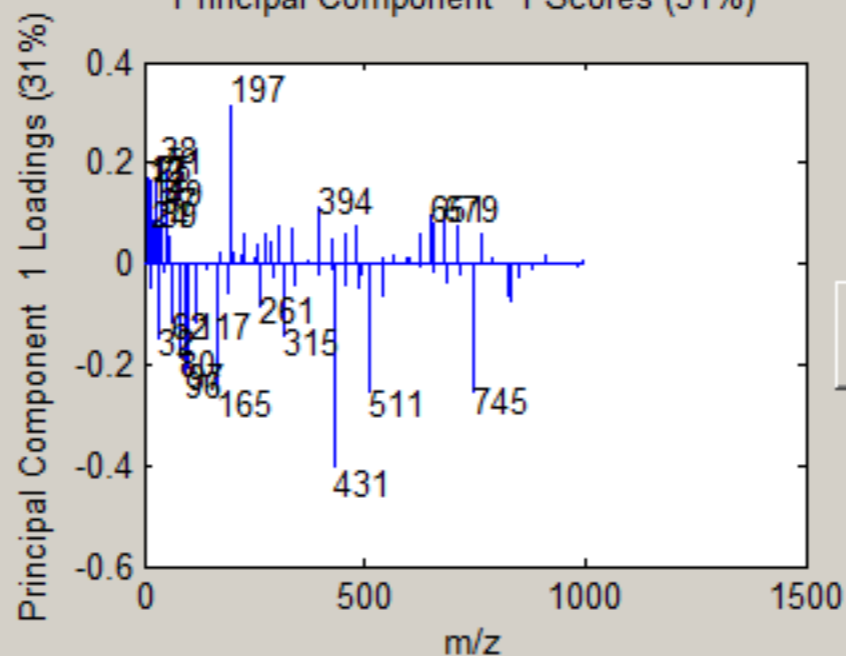
Y-Axis

And the 'Plot Loads' button to update the Loadings plot.

Plot Loads



EXT Plot



EXT Plot

Save PCA Data to Workspace

Number of PCs to keep

Scores output name

Loadings output name

Percent variance output name

Model output name

Save To Workspace

Close Panel

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.

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Load Selected Data

Data: **ndatat**
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 Variables: **exactmass**

Scaling Method

Run PCA

Show Eigenvalue Scree Plot

PCA Summary

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5	8.4	93.4
6	6.1	99.5
7	0.4	99.9
8	0.1	99.9
9	0	99.9
10	0	100

PCA Panel

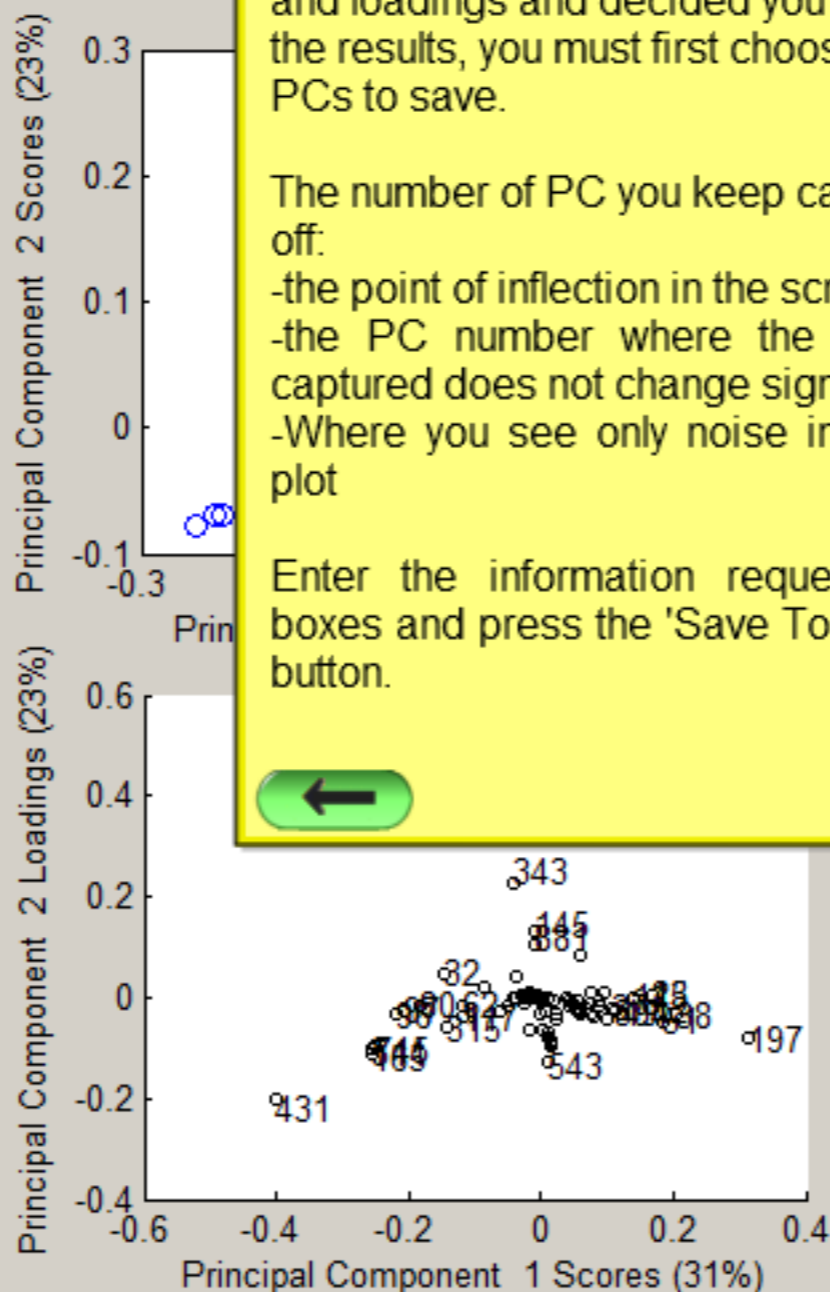
Plot PCA Scores and Loadings

These plots are for a quick check of the results and cannot be saved.

Loading plots default to m/z vs PC#.

X-Axis

Y-Axis



EXT Plot

Save PCA Data to Workspace

Number of PCs to keep

Scores output name

Loadings output name

Percent variance output name

Model output name

Save To Workspace

Close Panel

Once you have browsed the PCA scores and loadings and decided you want to save the results, you must first choose how many PCs to save.

The number of PC you keep can be based off:

- the point of inflection in the scree plot
- the PC number where the % variance captured does not change significantly
- Where you see only noise in the scores plot

Enter the information requested in the boxes and press the 'Save To Workspace' button.

Name	Value
data	<42x84 double>
exactmass	<84x15 char>
filenames	<42x15 char>
labels	<84x15 char>
loads	<84x4 double>
model	<1x1 struct>
ndatat	<42x84 double>
nommass	<84x3 char>
samplenames	<42x4 char>
scores	<42x4 double>
totalcounts	<42x1 double>
var	<4x4 double>

New to MATLAB? Watch this [Video](#), see [Demos](#), or read [Getting Started](#).

```
>> spectragui  
fx >> |
```

The data is saved to the workspace using the names provided.



Data Selection Panel

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8	0.1	99.9
9	0	99.9
10	0	100

PCA Panel

Plot PCA Scores and Loadings

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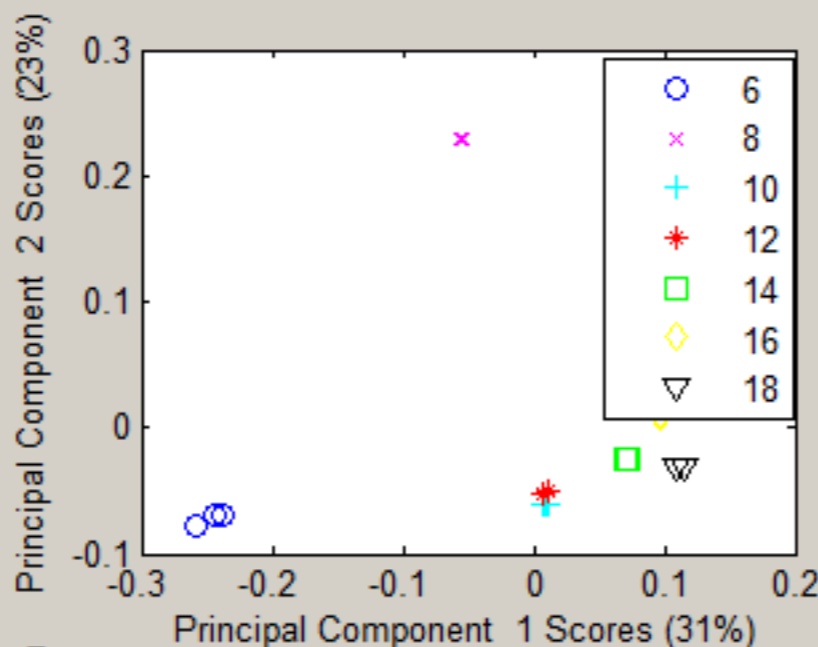
Loading plots default to m/z vs PC#.

X-Axis

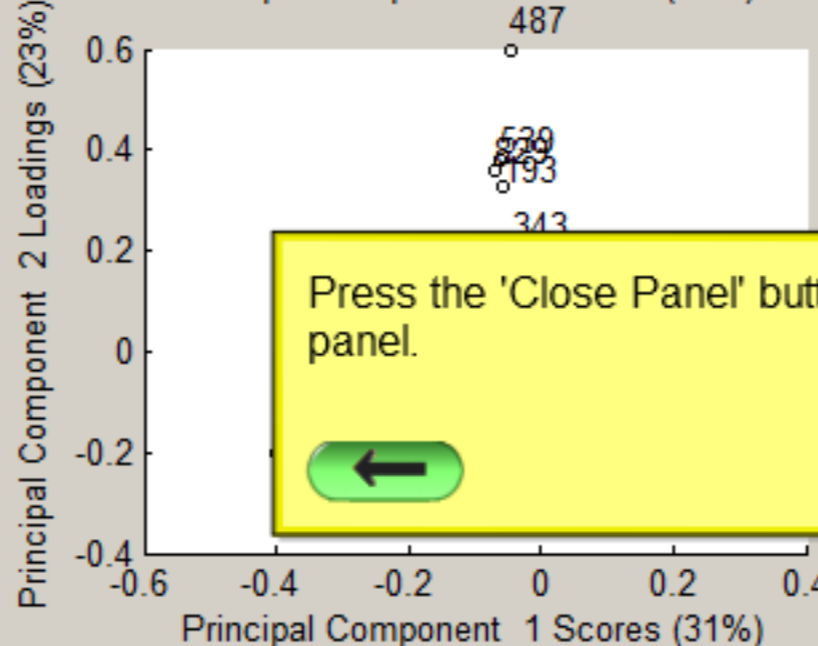
Y-Axis

Plot Scores

Plot Loads



EXT Plot



Save PCA Data to Workspace

Number of PCs to keep

Scores output name

Loadings output name

Percent variance output name

Model output name

Save To Workspace

Press the 'Close Panel' button to close the panel.

Close Panel

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

ndatat

Name of Variable Matrix

exactmass

Name of Filename Matrix

filenames

Name of Totalcounts Matrix

totalcounts

Name of Samplenames Matrix

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.

