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.
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.

This tutorial will show how to create and label a loadings plot.
From the 'Data Display' menu choose -> 'Plot Loadings'
Raw Data Selection Panel

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<table>
<thead>
<tr>
<th>Name of Data Matrix</th>
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<th>Name of Samplenames Matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>ndataset</td>
<td>exactmass</td>
<td>filenames</td>
<td>totalcounts</td>
<td>Select Samples</td>
</tr>
</tbody>
</table>

MVA Data Selection Panel

<table>
<thead>
<tr>
<th>Name of Scores Matrix</th>
<th>Name of Loadings Matrix</th>
<th>Name of % Variance Matrix</th>
<th>Name of Model Matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>scores</td>
<td>loads</td>
<td>variance</td>
<td>model</td>
</tr>
</tbody>
</table>

Plot Loadings

Load Selected Data

- Load Selected Data

Loaded Data

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

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MVA Data Selection Panel

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<td>loads</td>
<td>variance</td>
<td>model</td>
</tr>
</tbody>
</table>

Plot Loadings

Load Selected Data

- Load Selected Data

Loaded Data

- Loadings: loads
- Variables: exactmass
- % Variance: variance

PC# to plot

- 1

Press the 'Plot Loads' button
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.

MVA Data Selection Panel

Plot Loadings

The plot is created.
This plot can be saved at any time using the 'Save Figure' button above.
To label the loadings plot choose 'Label Loadings Plot' from the 'Data Display' Menu.
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.

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<td>variance</td>
<td>model</td>
</tr>
</tbody>
</table>

Plot Loadings

Load Selected Data

And press the 'Label Threshold' button.

Label Loadings

Label all peaks above a threshold value.

PO# to plot

1

Plot Loads

Save Figure

Use custom labels for selected peaks.

Turn Selection Mode ON/OFF

OFF

Custom Labels to use

Choose Peaks

Label Custom

Close Panel

Plot Raw Data Plot For Labeled Peaks
The peaks above this threshold value are labeled using the nominal mass value of the given peak.
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.
The figures are saved to the currently active Matlab directory.
The plots look like this.
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: mdatass
Name of Variable Matrix: exactmass
Name of Filename Matrix: filenames
Name of Totalcounts Matrix: totalcounts
Name of Sample names 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

PC# to plot: 1

Load Selected Data
Loaded Data

Label Loadings

Label all peaks above a threshold value.
Label Peaks Above
Label Threshold
Create Raw Data Plot For Labeled Peaks

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.
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.

MVA Data Selection Panel

Plot Loadings
Load Selected Data
Loaded Data

Label Loadings
Label all peaks above a threshold value.

Use custom labels for selected peaks.
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']
```
Note the spaces to keep the labels the same length.
Press <enter> to save the new variable to the workspace.
The new labels variable is created.
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: ndataset
- Name of Variable Matrix: exactmass
- Name of Filenames 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
- Loaded Data
- PC# to plot

Label Loadings

Label all peaks above a threshold value.

- Label Peaks Above
- Label Threshold
- Create Raw Data Plot for Labeled Peaks

Align the cross hairs on the desired peak and click on the peak(s) you want to label. The number of peaks you select has to equal the number of labels you created.

For this tutorial I created 4 labels, so I need to select 4 peaks.

The numbers on the following 4 slides are part of the tutorial and will not show up when you select peaks.

Use custom labels for selected peaks.

- Custom Labels to use
- Choose Peaks
- Label Custom

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: ndatas
- 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: nowmodel

Plot Loadings

- Load Selected Data
- Loaded Data
- Loadings: newloads
- Variables: exactmass
- % Variance: newvar

PC# to plot: 1

Label Loadings

- Label all peaks above a threshold value.
- Label Peaks Above
- Label Threshold

Create Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

- Custom Labels to use
- Choose Peaks
- Label Custom

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: 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: nowmodel

Plot Loadings

Load Selected Data
Loaded Data

Load Selected Data

Loaded Data

PC# to plot

Plot Loads
Save Figure
Close Panel

Label Loadings

Label all peaks above a threshold value.

Label Peaks Above
Label Threshold

Create Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

Press the 'Label Custom' button.

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**: 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**: nowmodel

Plot Loadings

- **Load Selected Data**
  - **Load Selected Data**

Label Loadings

- **Label all peaks above a threshold value.**

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

Use custom labels for selected peaks.

- **Custom Labels to use**
  - customlabels
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.
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: mdatas
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

Load Selected Data
Load Selected Data

PC# to plot: 1

The file is saved where you put it and looks like this.

These Are These
Peaks Big

Principal Component 1 (60%)

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

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: ndat
- 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: scores
- Name of Loadings Matrix: loads
- Name of % Variance Matrix: var
- Name of Model Matrix: model

Plot Loadings

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

Label Loadings

Label all peaks above a threshold value.

- Label Peaks Above
- Label Threshold

Create Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

- Custom Labels to use
- Choose Peaks
- Label Custom

Close Panel

Plot of Principal Component 1 (31%)

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

MVA Data Selection Panel

Label Loadings
Label all peaks above a threshold value.

Use custom labels for selected peaks.

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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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.