

### 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.

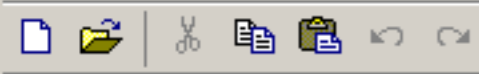


This is the 'Go to URL' button. It takes you to a website link.



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





Shortcuts How to Add What

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

```

This tutorial will show how to export the PCA data to text files.

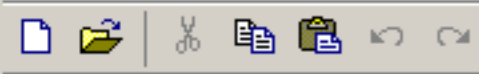
For this from the 'MVA' menu choose -> 'Export MVA Data'

These are the parameters for the analysis unless you specify otherwise. You can use the parameters you want to use in your analysis.

Name of Data Matrix:

Name of Totalcounts Matrix:

Name of Samplenames Matrix:



Workspace

Workspace panel showing a list of variables: Xdata, Ydata, data, exactmass, filenames, labeledpeaks, labels, loads, model, ndatass, nommass, samplenames, scores, totalcounts, variance.

Command History

Command History window showing a single command: `----%-- 10/5/10 10:04 A`

### 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 ndatass	Name of Variable Matrix Select Variables	Name of Filename Matrix filenames	Name of Totalcounts Matrix totalcounts	Name of Samplenames Matrix Select Samples
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### MVA Data Selection Panel

Name of Scores Matrix scores	Name of Loadings Matrix Select Loadings	Name of % Variance Matrix Select %Variance	Name of Model Matrix model
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### Save PCA data to files

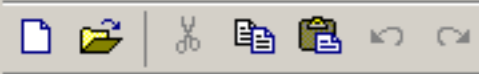
Load Selected Data

Scores:	None
Loadings:	None
Variance:	None
Variables:	None
Filenames:	None

Save PCA Data

Close Panel

Yellow callout box with text: "Make sure the correct data is loaded in the drop down menus in the 'Raw Data Selection Panel' and the 'MVA Data Selection Panel' and press the 'Load Selected Data' button." Below the text are two green arrow buttons pointing left and right.



Workspace

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

Command History

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

### 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 <input type="text" value="ndatass"/>	Name of Variable Matrix <input type="text" value="exactmass"/>	Name of Filename Matrix <input type="text" value="filenames"/>	Name of Totalcounts Matrix <input type="text" value="totalcounts"/>	Name of Samplenames Matrix <input type="text" value="Select Samples"/>
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### MVA Data Selection Panel

Name of Scores Matrix <input type="text" value="scores"/>	Name of Loadings Matrix <input type="text" value="loads"/>	Name of % Variance Matrix <input type="text" value="variance"/>	Name of Model Matrix <input type="text" value="model"/>
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### Save PCA data to files

Load Selected Data

Scores: **scores**  
 Loadings: **loads**  
 Variance: **variance**  
 Variables: **exactmass**  
 Filenames: **filenames**

Save PCA Data

Close Panel

Press the 'Save PCA Data' Button and choose where you want to save the data from the dialog that opens up.

← →

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

```

### 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: **ndatass**    Name of Variable Matrix: **exactmass**    Name of Filename Matrix: **filenames**    Name of Totalcounts Matrix: **totalcounts**    Name of Samplenames Matrix: **Select Samples**

### MVA Data Selection Panel

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

### Save PCA data to files

**Load Selected Data**

Scores: **scores**  
 Loadings: **loads**  
 Variance: **variance**  
 Variables: **exactmass**  
 Filenames: **filenames**

**Save PCA Data**

**Close Panel**

### Browse For Folder

Location to save files

- R2006b
  - bin
  - demos
  - extern
  - help
  - ja
  - java
  - jhhelp
  - notebook
  - sys
  - toolbox
  - uninstall
  - work
- McAfee
- MDL ISIS Draw 2.5
- Messenger
- Microsoft ActiveSync

Folder OK Cancel

Select the folder where you want to save the files.  
This can be any directory you want.

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

```

### 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: **ndatass**    Name of Variable Matrix: **exactmass**    Name of Filename Matrix: **filenames**    Name of Totalcounts Matrix: **totalcounts**    Name of Samplenames Matrix: **Select Samples**

### MVA Data Selection Panel

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

### Save PCA data to files

**Load Selected Data**

Scores: **scores**  
 Loadings: **loads**  
 Variance: **variance**  
 Variables: **exactmass**  
 Filenames: **filenames**

**Save PCA Data**

**Close Panel**

### Browse For Folder

Location to save files

- R2006b
  - bin
  - demos
  - extern
  - help
  - ja
  - java
  - help
- McAfee
- MDL ISIS Draw 2.0
- Messenger
- Microsoft ActiveSync

Make New Folder    **OK**    Cancel

Once you have selected where to save the data, press the 'Ok' button.

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

Name	Size	Type	Date Modified
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
S103.BIF	3,202 KB	BIF File	3/18/2010 4:57 PM
S11P3.BIF	7,428 KB	BIF File	8/17/2010 10:48 AM
S11P2.BIF	7,428 KB	BIF File	8/17/2010 10:47 AM
	7,428 KB	BIF File	8/17/2010 10:45 AM
	11,557 KB	BIF File	8/18/2010 8:31 AM
	7,428 KB	BIF File	8/17/2010 10:49 AM
	21,763 KB	BIF File	9/8/2010 1:40 PM
	12,290 KB	BIF File	9/9/2010 4:04 PM
	10,114 KB	BIF File	9/9/2010 3:34 PM
	5,443 KB	BIF File	9/8/2010 1:38 PM
	2,946 KB	BIF File	9/8/2010 2:57 PM
	21,763 KB	BIF File	9/8/2010 1:42 PM
	10,114 KB	BIF File	9/9/2010 3:43 PM
	12,290 KB	BIF File	9/9/2010 4:06 PM
	7,492 KB	BIF File	3/2/2010 3:31 PM
	112,012 KB	BIF File	1/4/2010 4:48 PM
	18,050 KB	BIF File	7/8/2010 1:24 PM
	3,841 KB	BIF File	9/2/2010 10:41 AM
	3,841 KB	BIF File	9/2/2010 10:41 AM
	2,817 KB	BIF File	1/4/2010 4:48 PM
	4,097 KB	BIF File	9/2/2010 10:24 AM
	4,097 KB	BIF File	9/2/2010 10:24 AM
	16,898 KB	BIF File	5/11/2010 9:00 AM
	3,8		
B4.BIF			
B1N.BIF			
A4.BIF			
3D_NEG.BIF			
1TEST.BIF			
codeforzoffsetsfg.asv			
variance.txt			
scores.txt			
loads_rescaled.txt			
loads.txt			

The data is saved into 4 text files.

variance.txt contains the % variance captured for each PC in the saved model.

scores.txt contains the scores for each PC in the saved model.

loads.txt contains the loadings for each PC in the saved model.

loads\_rescaled.txt contains the loadings where the x axis has been rescaled so that the loadings are plotted against a mass axis (m/z). This enables plotting the loadings so they look more like a mass spectrum.

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.

