

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.

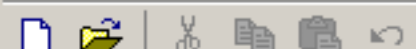


This is the 'Go to URL' button. It takes you to a website link.



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





Workspace



Name

data
exactmass
filenames
ndatass
nommass
samplenames
totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

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

This tutorial will cover how to run DPCA on your data using the spectragui.

This method is based on the paper: Yandle and Macfie in J. Chemometrics, v. 3, p. 589-600 (1989) and the code was adapted from code kindly provided by Matt Wagner PhD.

The data is automatically mean centered within this function.

No support of this function is provided.

It is included because I had the code for it.





Shortcuts How to Add

Workspace

- Name
- data
- exactmass
- filenames
- ndatass
- nommass
- samplenames
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

- Run PCA
- PCA Modelling
- Run DPCA
- Export MVA Data

From the 'MVA' menu choose -> Run DPCA

Name of Data Matrix

ndatass

Name of Variable

exactmass

Name of Totalcounts Matrix

totalcounts

Name of Samplenames Matrix

samplenames



Shortcuts [?] How to Add [?]

Workspace

- Name ▲
- data
- exactmass
- filenames
- ndatass
- nommass
- samplenames
- totalcounts

Current Directory Workspace

Command History

```

---%-- 10/8/10 10:49

```

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

PCA Panel

Input Information

Make sure the data you want to use is selected in the menus of the 'Data Selection Panel'.

←
→

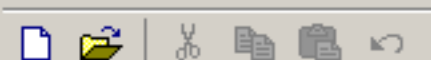
Data: None

Samples: None

Variables: None

DPCA Summary

PC#	%Var	%Vartotal



Shortcuts How to Add

Workspace



Name
data
exactmass
filenames
ndatass
nommass
samplenames
totalcounts

Current Directory Workspace

Command History

```
---%-- 10/8/10 10:49
```

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

DPCA 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

Then press the 'Load Selected Data' button.

← →

Data:	None
Samples:	None
Variables:	None

Run DPCA

Show Eigenvalue Scree Plot

DPCA Summary

PC#	%Var	%Vartotal
-----	------	-----------

Close Panel



Shortcuts How to Add

Workspace

Name ▲

- data
- exactmass
- filenames
- ndatass
- nommass
- samplenames
- totalcounts

Current Directory | Workspace

Current Directory Workspace

Command History

```

---%-- 10/8/10 10:49

```



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

DPCA 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: ndatass
Samples: samplenames
Variables: exactmass

Run DPCA

Once the data is loaded, press the 'Run DPCA' button.

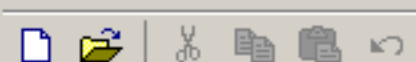
← →

Show Eigenvalue Scree Plot

DPCA Summary

PC#	%Var	%Vartotal

Close Panel



Shortcuts How to Add

Workspace



Name

- data
- exactmass
- filenames
- ndatass
- nommass
- samplenames
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

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:

DPCA Panel

Input Information

Make sure the data selected above is the data you want to analyze and then press

New panels that allow you to plot and save the DPCA data appear.

Samples: **samplenames**
Variables: **exactmass**

Run DPCA

Show Eigenvalue Scree Plot

DPCA Summary

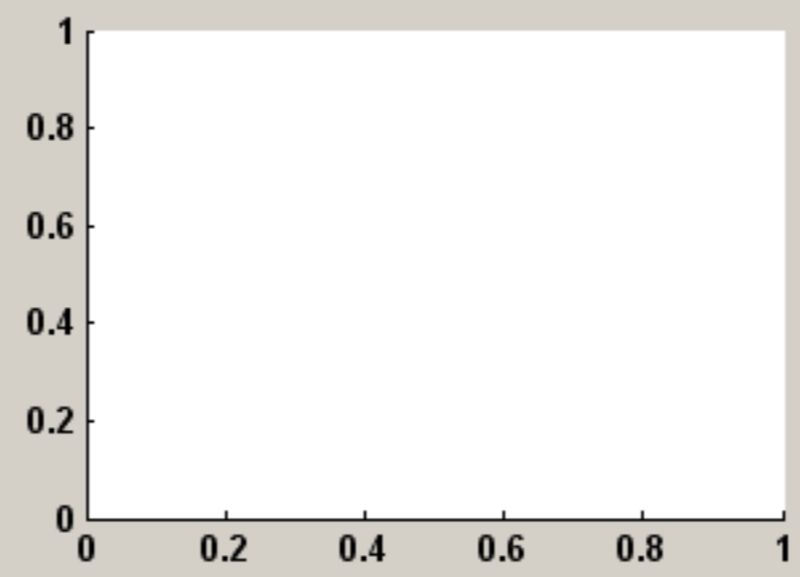
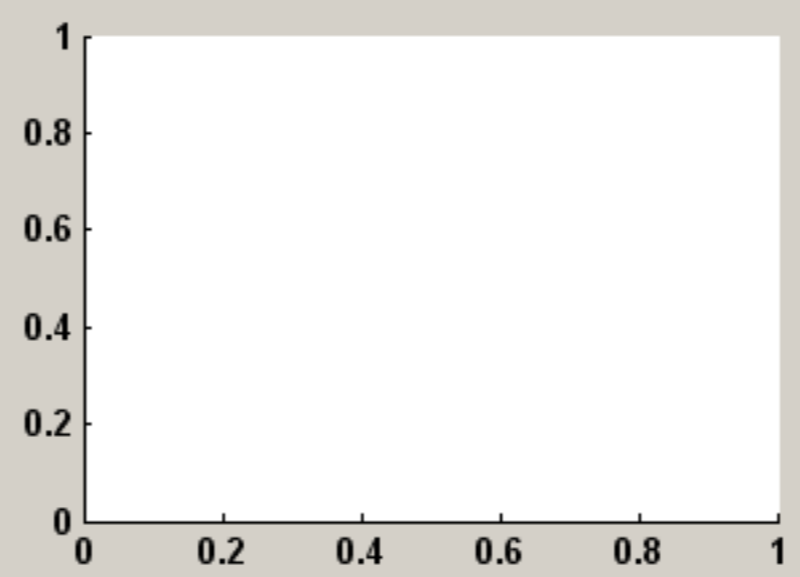
PC#	%Var	%Vartotal
1	52	52
2	19.5	71.5
3	12.6	84
4	8	92
5	4.3	96.3
6	3.7	100
7	0	100
8	0	100
9	0	100
10	0	100

Plot DPCA 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#.

PC# PC#



Save DPCA 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



Shortcuts How to Add

Workspace



Name

- data
- exactmass
- filenames
- ndatass
- nommass
- samplenames
- totalcounts

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:

DPCA Panel

Input Information

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

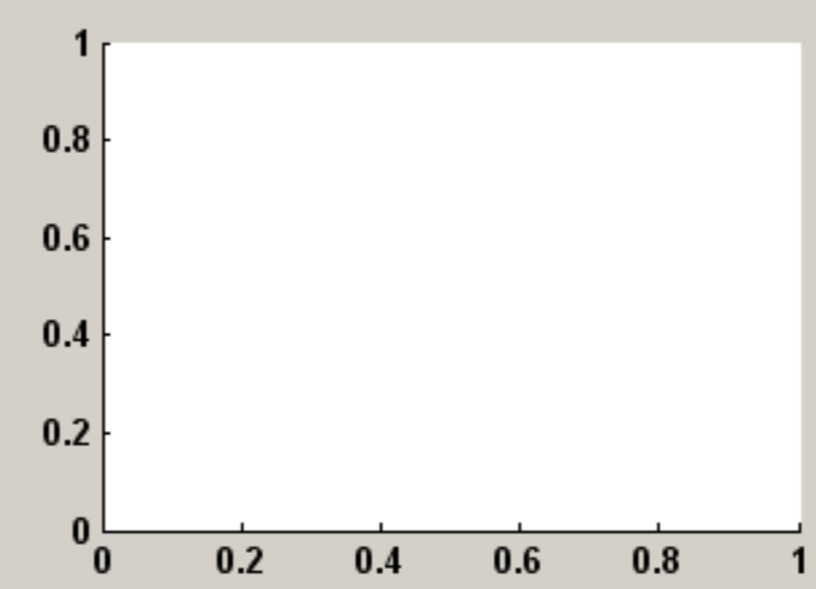
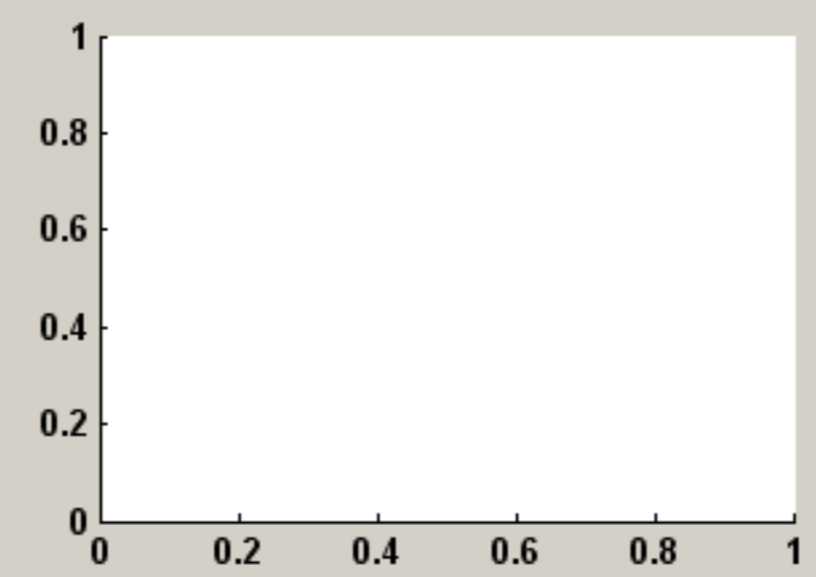
Data: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

Plot DPCA 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#.

Loading plots default to m/z vs PC#.

PC# PC#



Save DPCA Data to Workspace

Number of PCs to keep

Scores output name

Loadings output name

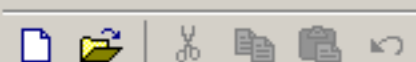
Percent variance output name

Model output name

A summary of the percent variance captured for each PC is shown in this table.

DPCA Summary

PC#	%Var	%Vartotal
1	52	52
2	19.5	71.5
3	12.6	84
4	8	92
5	4.3	96.3
6	3.7	100
7	0	100
8	0	100
9	0	100
10	0	100



Shortcuts How to Add

Workspace



Name

- data
- exactmass
- filenames
- ndatass
- nommass
- samplenames
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

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:

DPCA 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: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

Run DPCA

Show Eigenvalue Scree Plot

DPCA Summary

PC#	%Var	%Vartotal
1	52	52
2	19.5	71.5
3	12.6	84
4	8	92
5	4.3	96.3
6	3.7	100
7	0	100
8	0	100
9	0	100
10	0	100

Plot DPCA Scores and Loadings

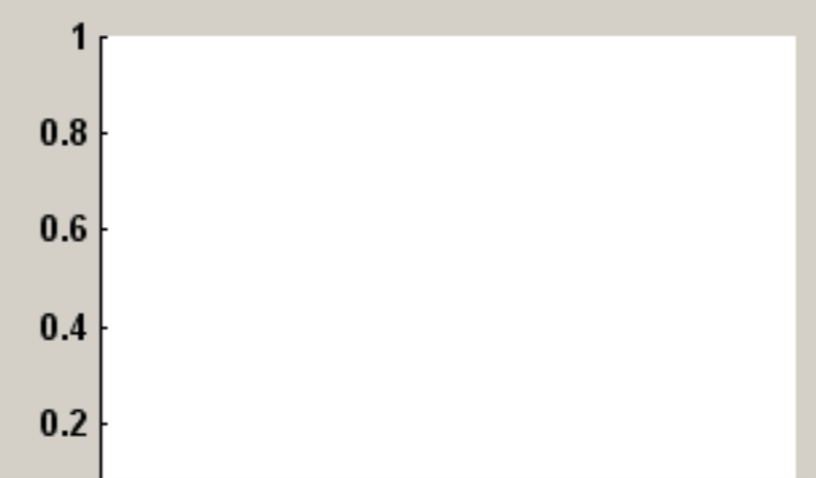
These plots are for a quick check of the results and cannot be saved.
Loading plots default to m/z vs PC#.

Loading plots default to m/z vs PC#.

PC# PC#

Plot Scores

Plot Loads



Save DPCA 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

To see a scree plot of the eigenvalues, press the 'Show Eigenvalue Scree Plot'

← →



Shortcuts [How to Add](#)

Workspace



Name ▲

- data
- exactmass
- filenames
- ndatass
- nommass
- samplenames
- totalcounts

Current Directory Workspace

Command History

```
---%-- 10/8/10 10:49
```

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:

DPCA Panel

Input Information

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

Data: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

Plot DPCA 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#.

Loading plots default to m/z vs PC#.

PC# PC#



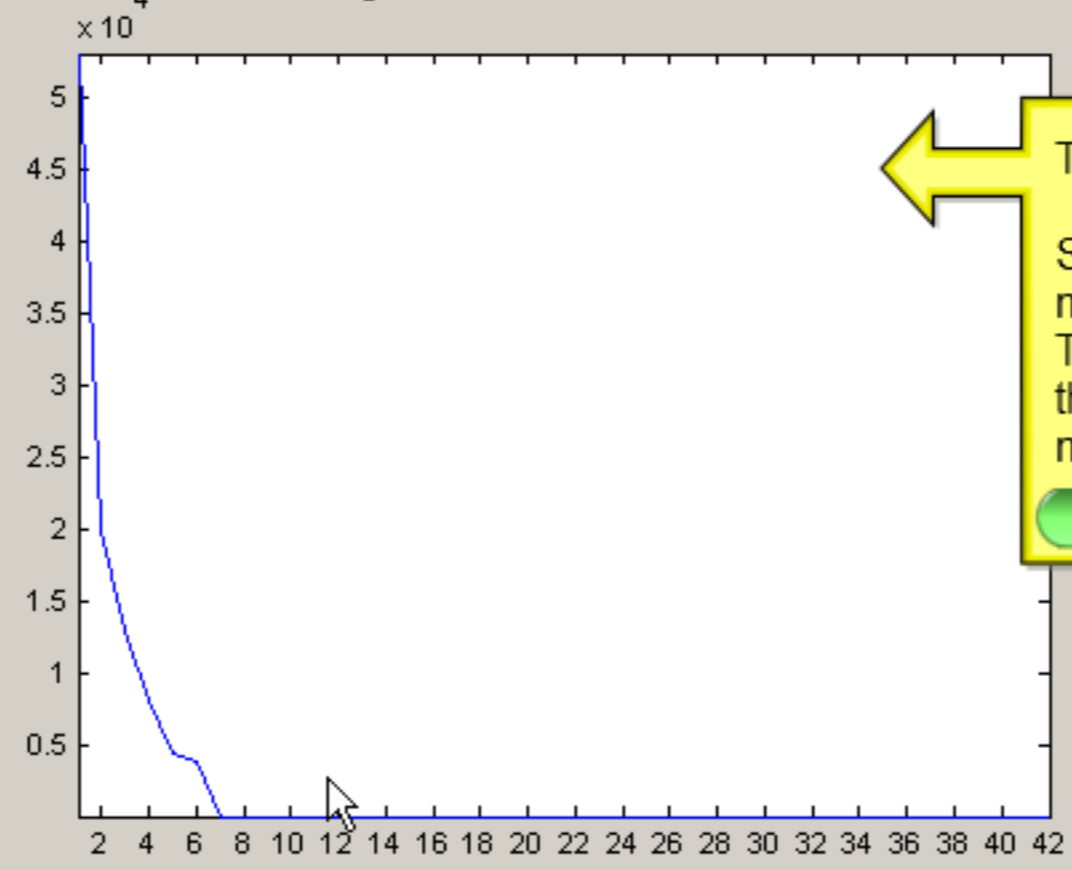
Save DPCA Data to Workspace

Number of PCs to keep:
 Scores output name:
 Loadings output name:
 Percent variance output name:

DPCA Summary

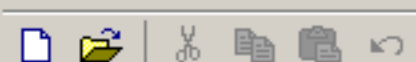
PC#	%Var	%Vartotal
1	52	52
2	19.5	71.5
3	12.6	84
4	8	92
5	4.3	96.3
6	3.7	100
7	0	100
8	0	100
9	0	100
10	0	100

Eigenvalue Scree Plot



The plot appears here.

Some people use this plot to determine how many PCs to keep within a model. Typically you look for points of inflection in the curve, or where the curve hits a minimum.



Shortcuts How to Add

Workspace



Name

- data
- exactmass
- filenames
- ndatass
- nommass
- samplenames
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

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**

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: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

Run DPCA

Show Eigenvalue Scree Plot

DPCA Summary

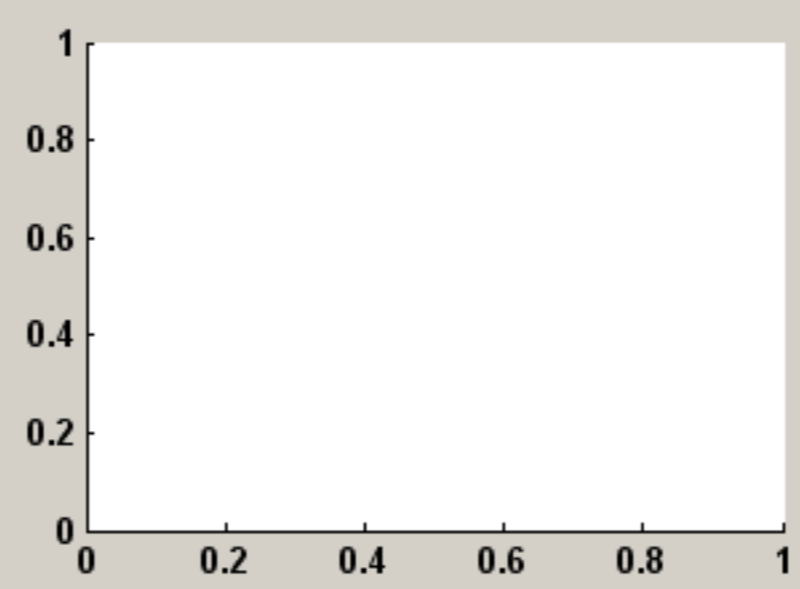
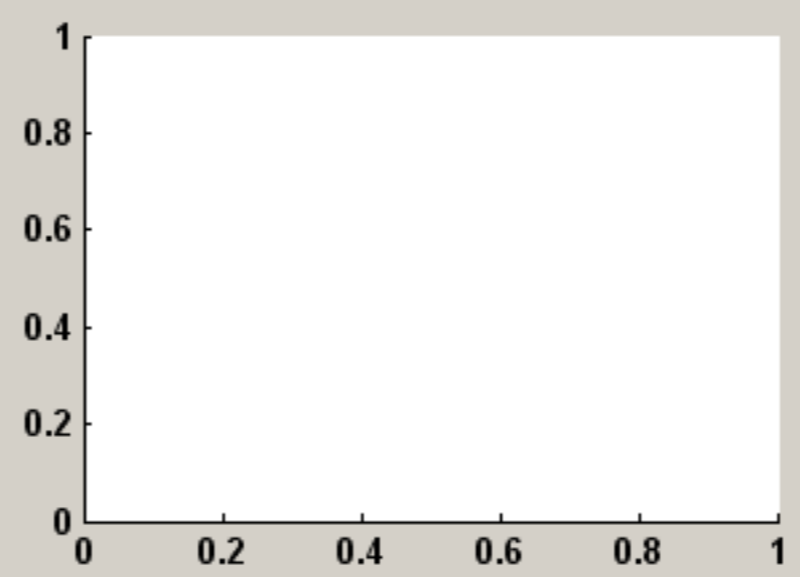
PC#	%Var	%Vartotal
1	52	52
2	19.5	71.5
3	12.6	84
4	8	92
5	4.3	96.3
6	3.7	100
7	0	100
8	0	100
9	0	100
10	0	100

DPCA Panel

Plot DPCA 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#.

PC# [] PC# []
 Plot Scores Plot Loads



Save DPCA Data to Workspace

Number of PCs to keep

You can create scores and loadings plots using this panel.
 These plots are intended to allow you to browse the results and cannot be saved.

Percent variance output name

Model output name

Save To Workspace

Close Panel



Shortcuts [How to Add](#)

Workspace



Name ▲

- data
- exactmass
- filenames
- ndatass
- nommass
- samplenames
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

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: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

Run DPCA

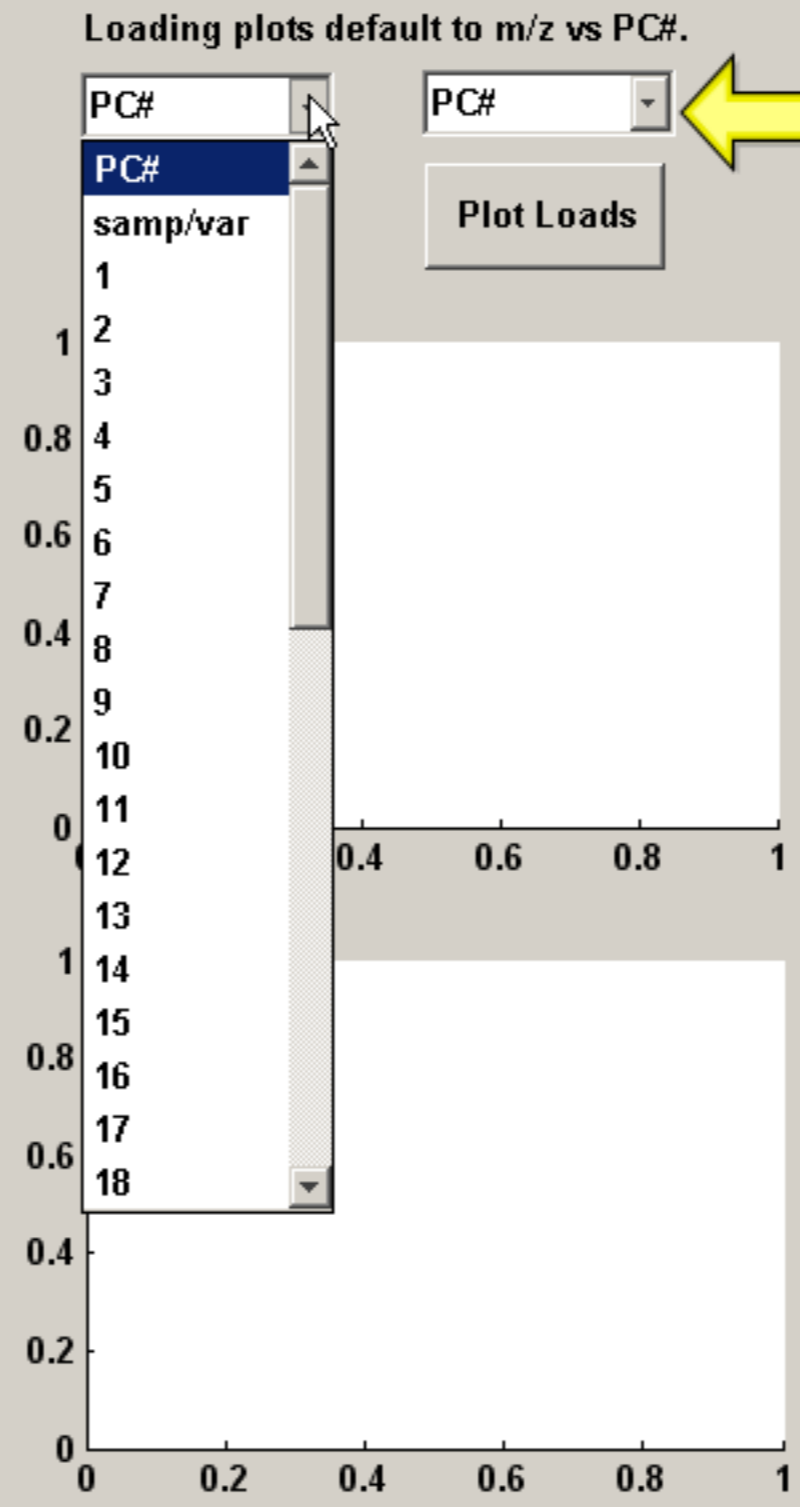
Show Eigenvalue Scree Plot

DPCA Summary

PC#	%Var	%Vartotal
1	52	52
2	19.5	71.5
3	12.6	84
4	8	92
5	4.3	96.3
6	3.7	100
7	0	100
8	0	100
9	0	100
10	0	100

DPCA Panel

Plot DPCA 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#.



PC#

Choose what you want to plot from the drop down menus.

The menu on the left is the x-axis, the menu on the right is the y-axis.

All loadings plots are plotted as the chosen PC number from the y-axis list vs m/z. The spectragui does not support plotting a cross plot of two PC loadings.

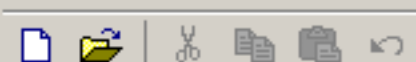
Save DPCA Data to Workspace

Number of PCs to keep

Model output name

Save To Workspace

Close Panel



Shortcuts How to Add

Workspace



Name

- data
- exactmass
- filenames
- ndatass
- nommass
- samplenames
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

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:

DPCA 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: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

Run DPCA

Show Eigenvalue Scree Plot

DPCA Summary

PC#	%Var	%Vartotal
1	52	52
2	19.5	71.5
3	12.6	84
4	8	92
5	4.3	96.3
6	3.7	100
7	0	100
8	0	100
9	0	100
10	0	100

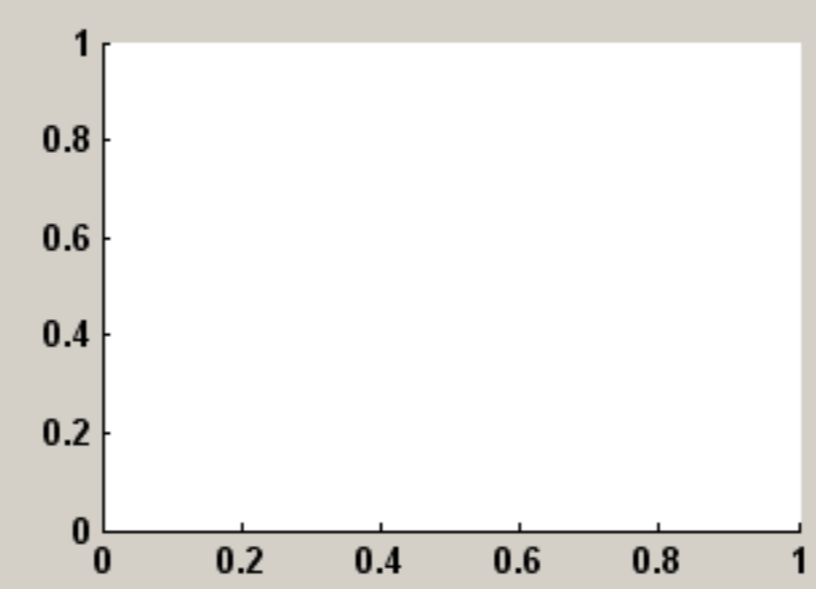
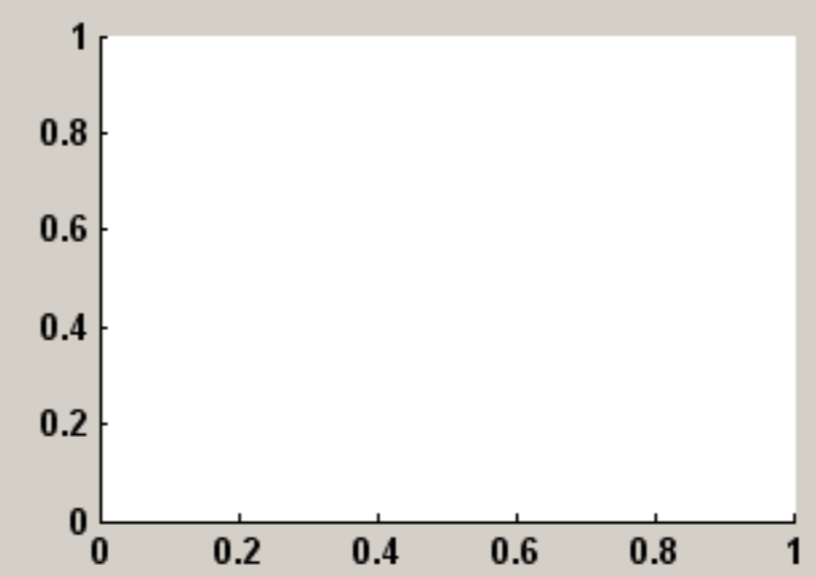
Plot DPCA Scores and Loadings

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

Loading plots default to m/z vs PC#.

Plot Scores

Plot Loads



Save DPCA Data to Workspace

Number of PCs to keep

After selecting what you want to plot, press the 'Plot Scores'



Percent variance output name

Model output name

Save To Workspace

Close Panel



Shortcuts [How to Add](#)

Workspace



Name ▲

- data
- exactmass
- filenames
- ndatass
- nommass
- samplenames
- totalcounts

Current Directory Workspace

Command History

```
---%-- 10/8/10 10:49
```

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.

Data: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

DPCA Summary

PC#	%Var	%Vartotal
1	52	52
2	19.5	71.5
3	12.6	84
4	8	92
5	4.3	96.3
6	3.7	100
7	0	100
8	0	100
9	0	100
10	0	100

DPCA Panel

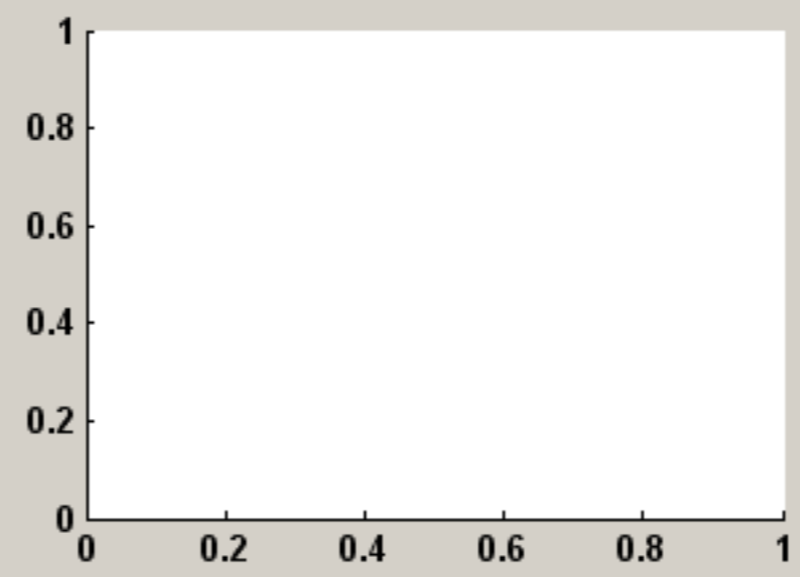
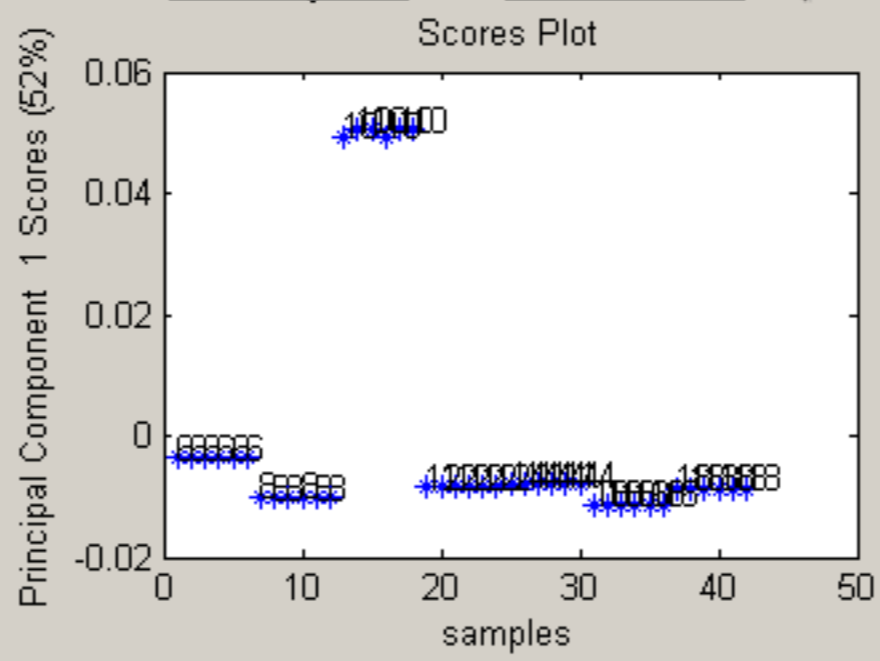
Plot DPCA Scores and Loadings

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

Loading plots default to m/z vs PC#.

samp/var: 1

And then 'Plot Loads' to create the plots.



Save DPCA Data to Workspace

Number of PCs to keep

Percent variance output name

Model output name



Shortcuts [How to Add](#)

Workspace



Name ▲

- data
- exactmass
- filenames
- ndatass
- nommass
- samplenames
- totalcounts

Current Directory Workspace

Command History

```
---%-- 10/8/10 10:49
```

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: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

Run DPCA

Show Eigenvalue Scree Plot

DPCA Summary

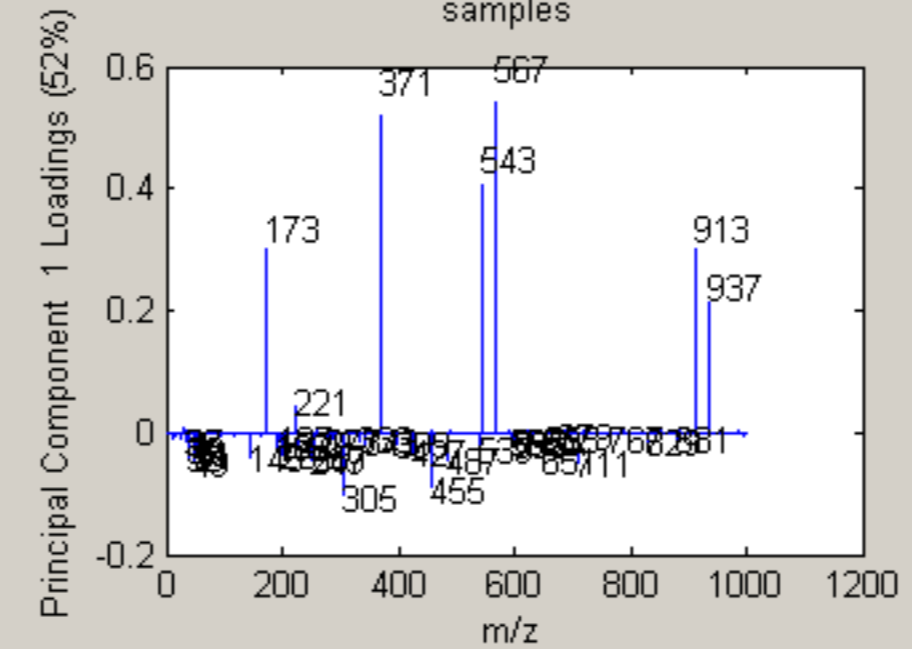
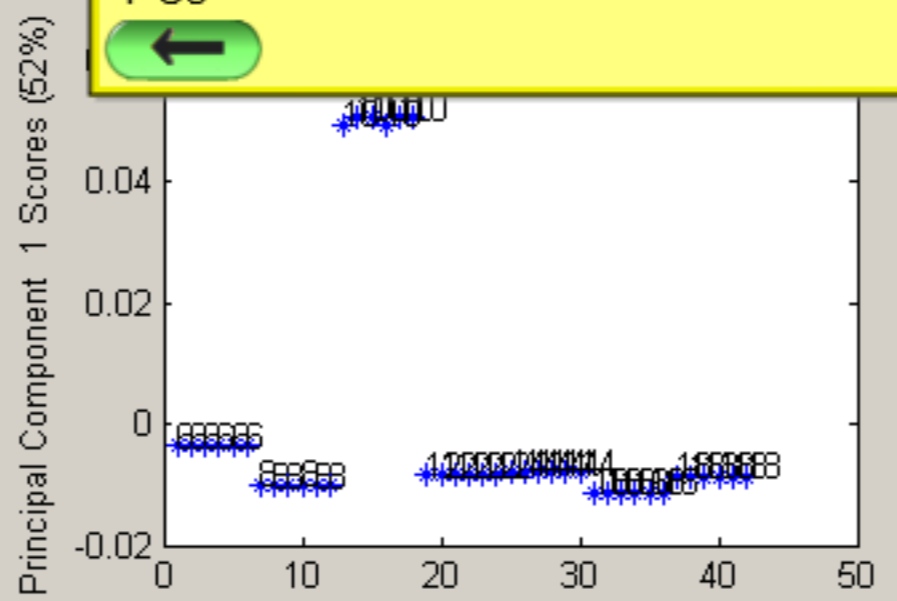
PC#	%Var	%Vartotal
1	52	52
2	19.5	71.5
3	12.6	84
4	8	92
5	4.3	96.3
6	3.7	100
7	0	100
8	0	100
9	0	100
10	0	100

DPCA Panel

Plot DPCA Scores and Loadings

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

Once you are happy with the results type the number of PCs you would like to keep in the saved data here. This can be any number up to the maximum number of PCs



Save DPCA Data to Workspace

Number of PCs to keep:

Scores output name:

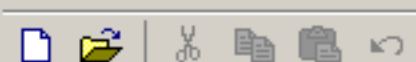
Loadings output name:

Percent variance output name:

Model output name:

Save To Workspace

Close Panel



Shortcuts [How to Add](#)

Workspace



Name ▲

- data
- exactmass
- filenames
- ndatass
- nommass
- samplenames
- totalcounts

Current Directory Workspace

Command History

---%-- 10/8/10 10:49

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.

Data: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

DPCA Summary

PC#	%Var	%Vartotal
1	52	52
2	19.5	71.5
3	12.6	84
4	8	92
5	4.3	96.3
6	3.7	100
7	0	100
8	0	100
9	0	100
10	0	100

DPCA Panel

Plot DPCA Scores and Loadings

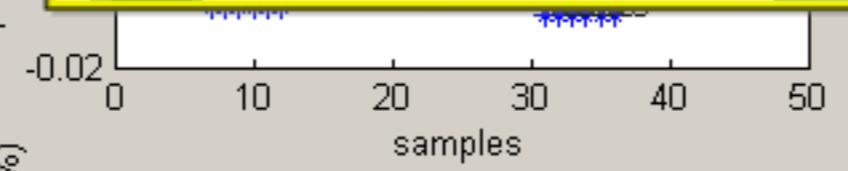
These plots are for a quick check of the results and cannot be saved. Loading plots default to m/z vs PC#.

Loading plots default to m/z vs PC#.

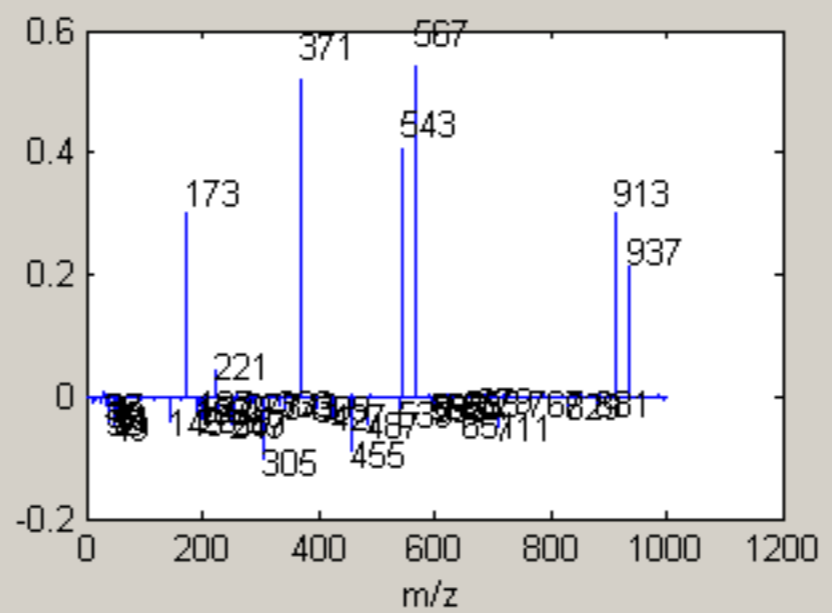
Next enter names for the scores, loadings, percent variance, and model in their respective boxes.

These names should be unique names to prevent overwriting data in the Matlab workspace.

Principal Component 1 Scores (52%)



Principal Component 1 Loadings (52%)



Save DPCA Data to Workspace

Number of PCs to keep

Scores output name

Loadings output name

Percent variance output name

Model output name



Shortcuts How to Add

Workspace



Name

- data
- exactmass
- filenames
- ndatass
- nommass
- samplenames
- totalcounts

Current Directory Workspace

Command History

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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: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

Run DPCA

Show Eigenvalue Scree Plot

DPCA Summary

PC#	%Var	%Vartotal
1	52	52
2	19.5	71.5
3	12.6	84
4	8	92
5	4.3	96.3
6	3.7	100
7	0	100
8	0	100
9	0	100
10	0	100

DPCA Panel

Plot DPCA Scores and Loadings

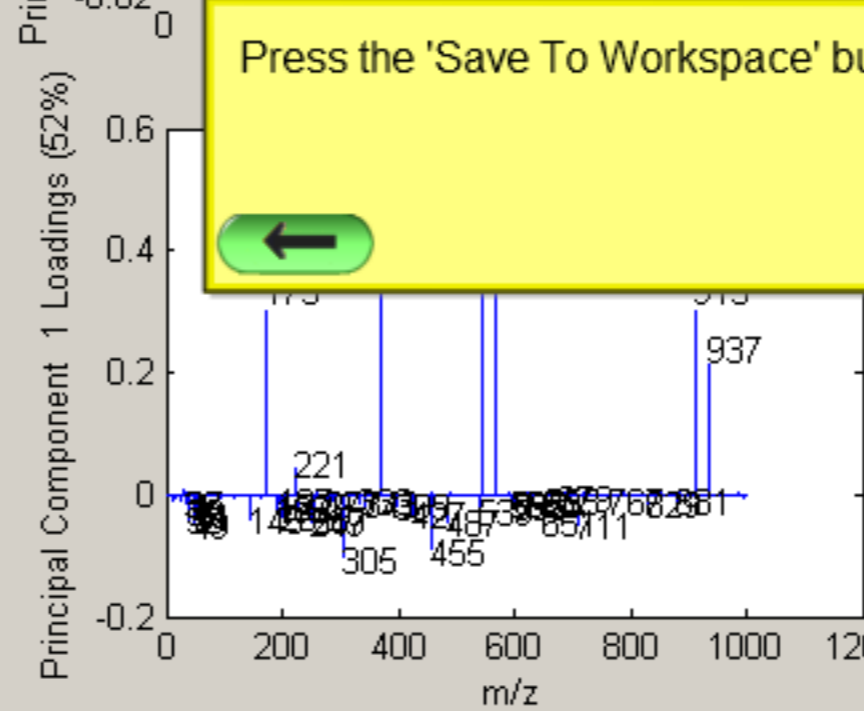
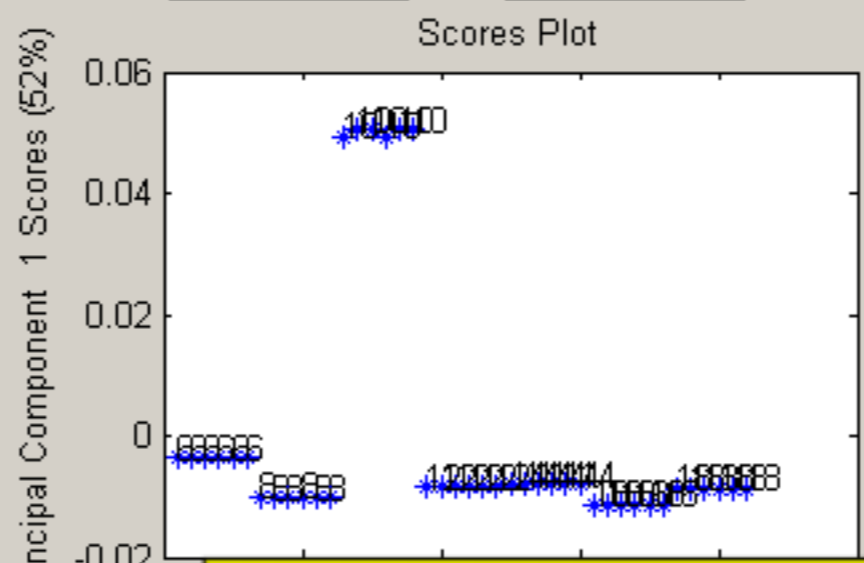
These plots are for a quick check of the results and cannot be saved.
 Loading plots default to m/z vs PC#.

Loading plots default to m/z vs PC#.

samp/var: 1

Plot Scores

Plot Loads



Save DPCA 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 'Save To Workspace' button.

Workspace

Name

- data
- dpcalloads
- dpcamodel
- dpcascores
- dpcavariance
- exactmass
- filenames
- ndatass
- nommass
- samplenames
- totalcounts

Current Directory Workspace

Command History

```

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```

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:

DPCA Panel

The data is saved to the Matlab workspace and entered into the respective drop down menus of the 'MVA Data Selection Panel'.

Plot DPCA Scores and Loadings

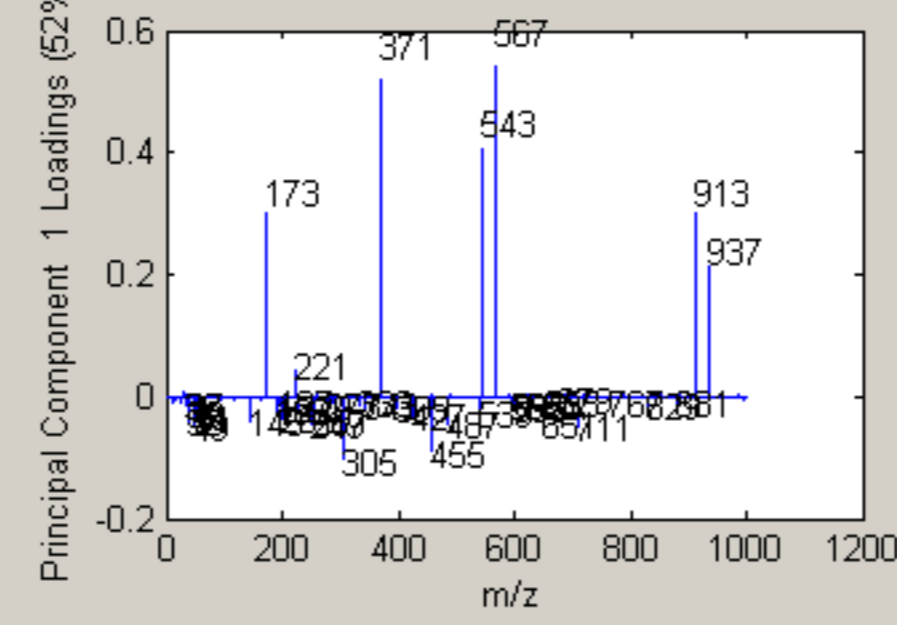
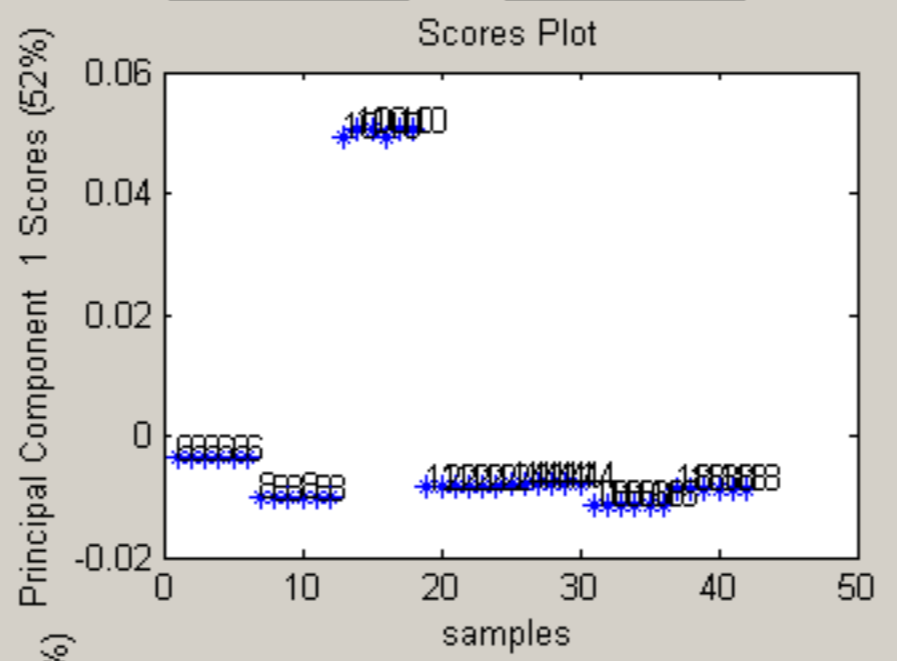
These plots are for a quick check of the results and cannot be saved. The default plotting plots default to m/z vs PC#.

Plotting:

Data: **ndatass**
 Samples: **samplenames**
 Variables: **exactmass**

DPCA Summary

PC#	%Var	%Vartotal
1	52	52
2	19.5	71.5
3	12.6	84
4	8	92
5	4.3	96.3
6	3.7	100
7	0	100
8	0	100
9	0	100
10	0	100



Save DPCA Data to Workspace

Number of PCs to keep:

Scores output name:

Loadings output name:

Percent variance output name:

Model output name:



Shortcuts How to Add

Workspace



- Name
- data
- dpcalloads
- dpcamodel
- dpcascores
- dpcavariance
- exactmass
- filenames
- ndatass
- nommass
- samplenames
- totalcounts

Current Directory Workspace

Command History

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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

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.

← →