

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
Select Totalcounts...

Name of Samplenames Matrix
samplegroups ...

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	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatassp	exactmass	filenames	Select Totalcounts	samplenames

This tutorial covers how to use a function called the PC Data browser. The function allows the user to look at pre processed data after subtracting previous PCs from a data set.

This function was created in order to look at the data that PCA is using when it calculates PCs after PC1. As illustrated in the figure on the right, each subsequent PC is calculated from the data matrix not captured by the previous PC. This means it is using the data matrix minus the previous PC.

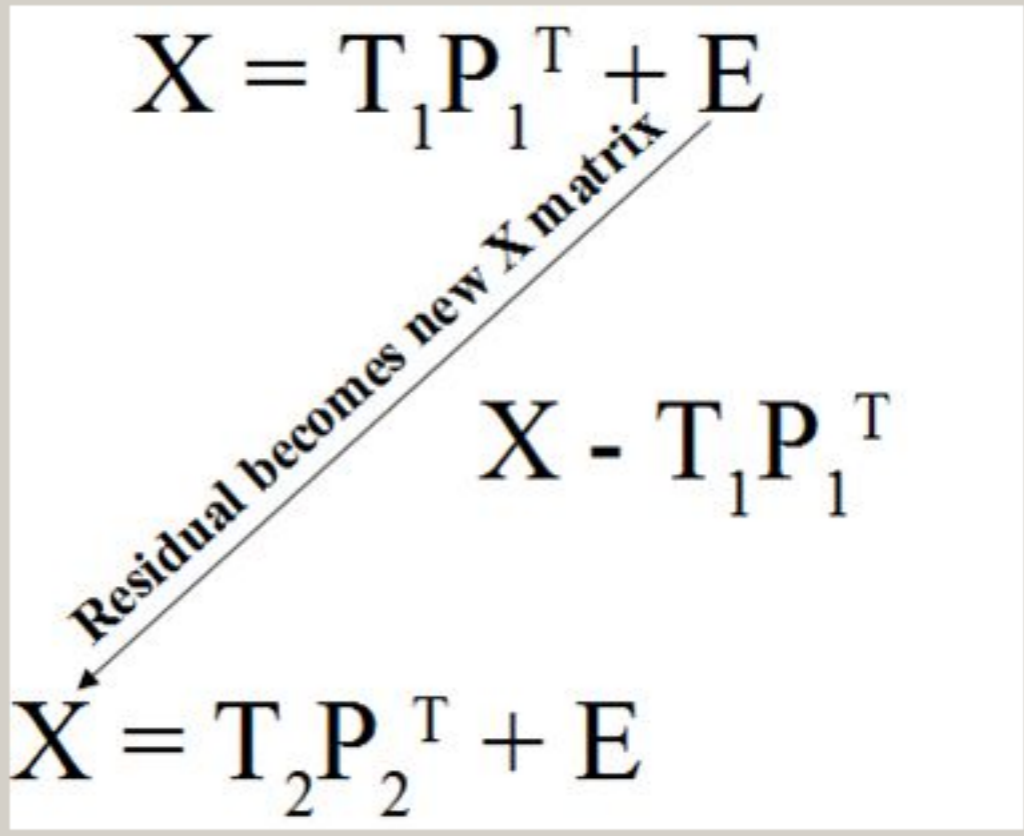
It is always recommended that one looks back at the "original" data when interpreting PCA results. This can be easily done for PC1, where even looking back at the non pre processed data will show trends similar to those seen in PCA. However for subsequent PCs one cannot look at the original data matrix and expect to see the trends shown in the PCA results.

In fact, one should really look at the pre processed data used for a given PC when looking at trends in the PCA results.

The PC Data browser enables this functionality and provides a way for the user to look at peak area images of the pre processed data for a given PC (pre processed matrix - previous PCs).

In this tutorial I will provide examples of how this works and why it can be useful.

← →



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

This tutorial assumes that you have already loaded some data (see tutorial 02/03/04), ran PCA and saved the PCA results (see tutorial 07).

- 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

data that will be used in further analysis unless you specify otherwise.
s to select the data and information you want to use in your analysis.

Name of Data Matrix

ndatassp

Name of Samplenames Matrix

samplenames

Select 'PC Data Browser' from the 'Data Display' menu.

← →

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="ndatassp"/>	<input type="text" value="exactmass"/>	<input type="text" value="filenames"/>	<input type="text" value="Select Totalcounts"/>	<input type="text" value="samplenames"/>

MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
<input type="text" value="scores"/>	<input type="text" value="loads"/>	<input type="text" value="var"/>	<input type="text" value="model"/>

Select the desired data from both the 'Data Selection Panel', and the 'MVA Data Selection Panel' above.

Choose score/loads/var a



Continue

Cancel

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
ndatassp	exactmass	filenames	Select 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

Choose score/loads/var above

Continue

After selecting the desired data. Press the 'Continue' 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	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
<input type="text" value="ndatassp"/>	<input type="text" value="exactmass"/>	<input type="text" value="filenames"/>	<input type="text" value="Select Totalcounts"/>	<input type="text" value="samplenames"/>

Load Selected Data

Then press the 'Load Selected Data' button.

Image: None
Variable: None
Scores: None
Loads: None

Data Preprocessing

PC #

Plot Scores and Loads

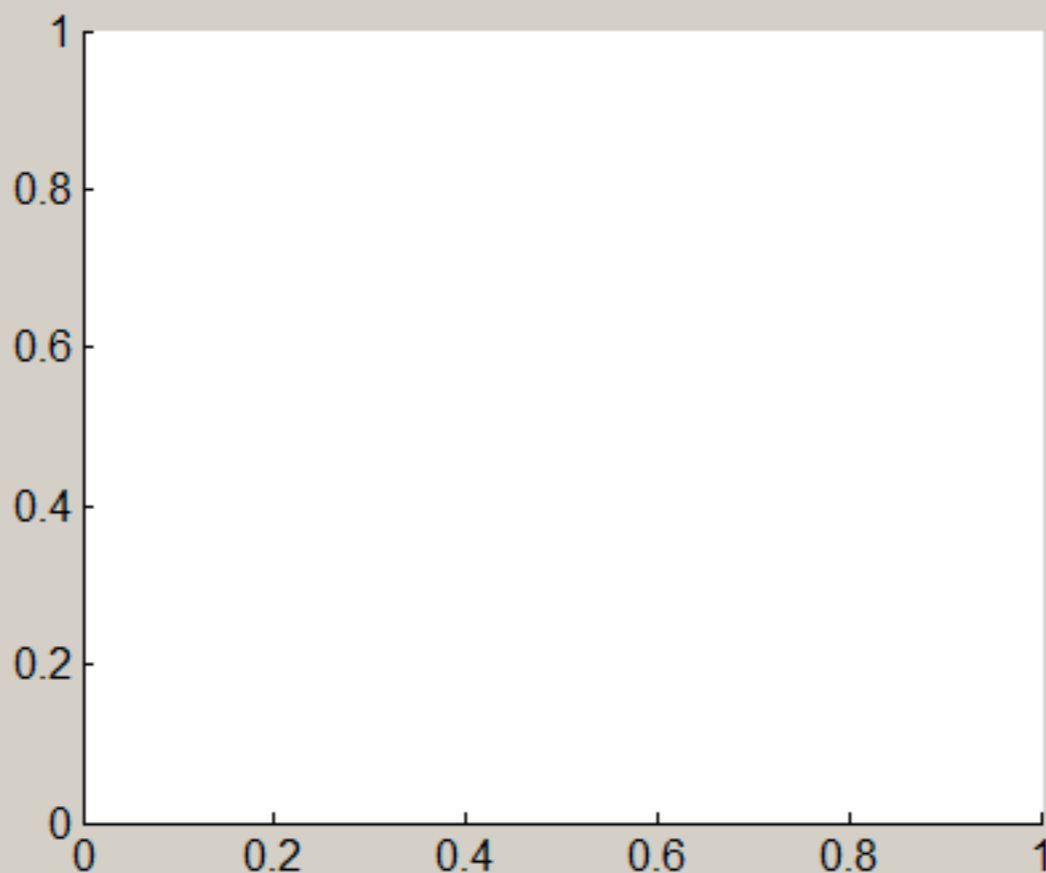
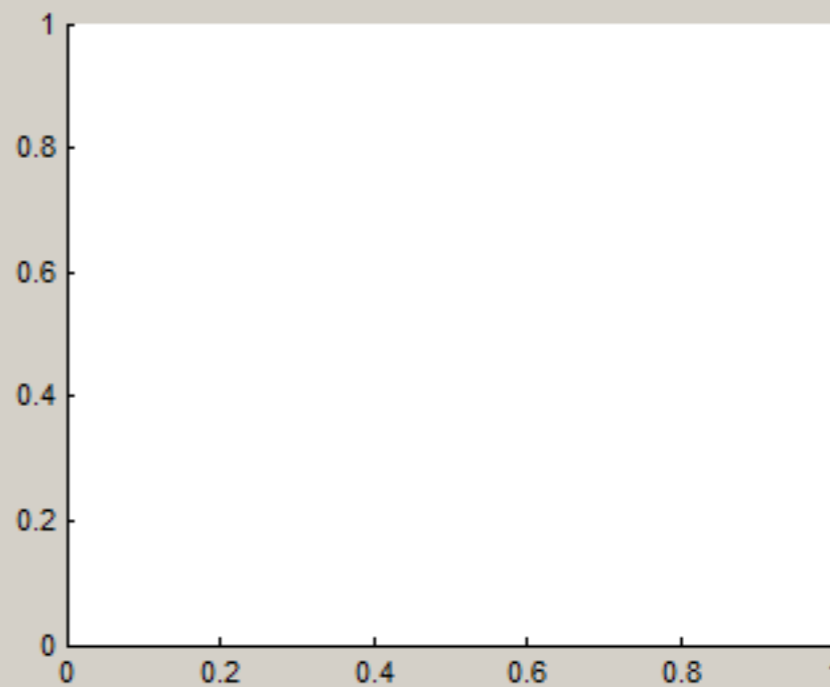
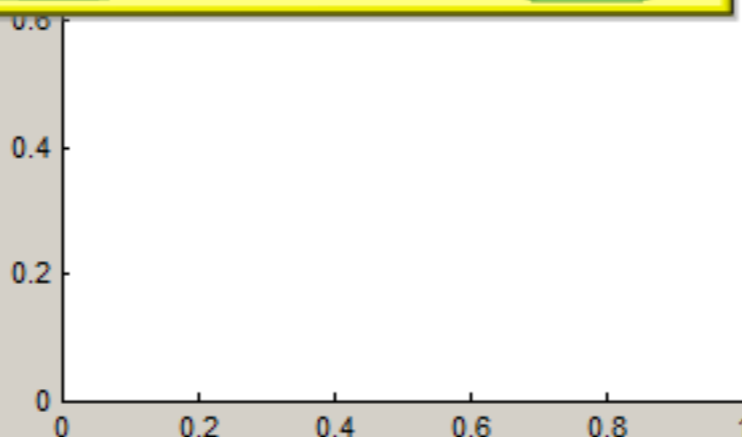
Peak List

--

Select Plot Type

Plot Peak Area Image

This plot will show the scaled for the selected peak after subtracting the PCs selected above.



Save Figure

Make Ext

Close Panel

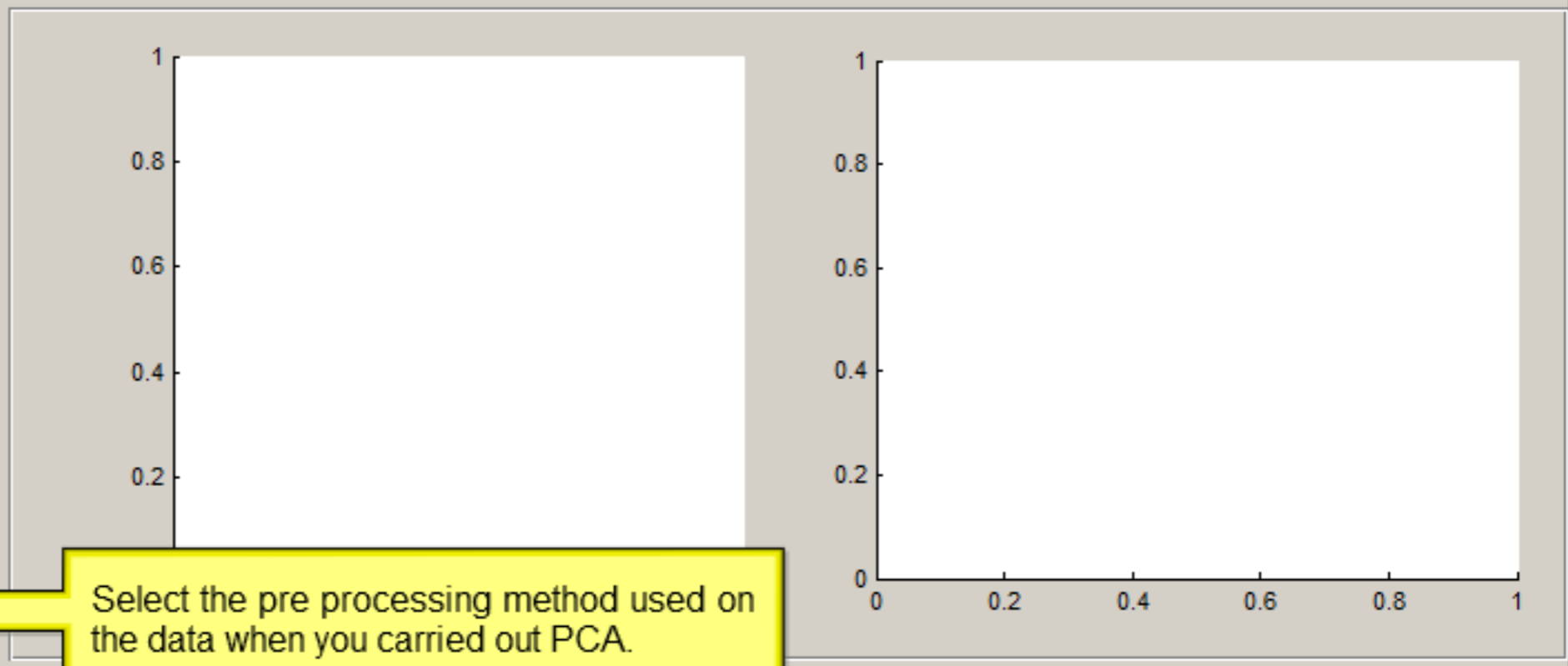
Data Selection Panel

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 <input type="text" value="ndatassp"/>	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="Select Totalcounts"/>	Name of Samplenames Matrix <input type="text" value="samplenames"/>
--	---	---	---	--

Load Selected Data

Image: **ndatassp**
Variable: **exactmass**
Scores: **scores**
Loads: **loads**



Data Preprocessing

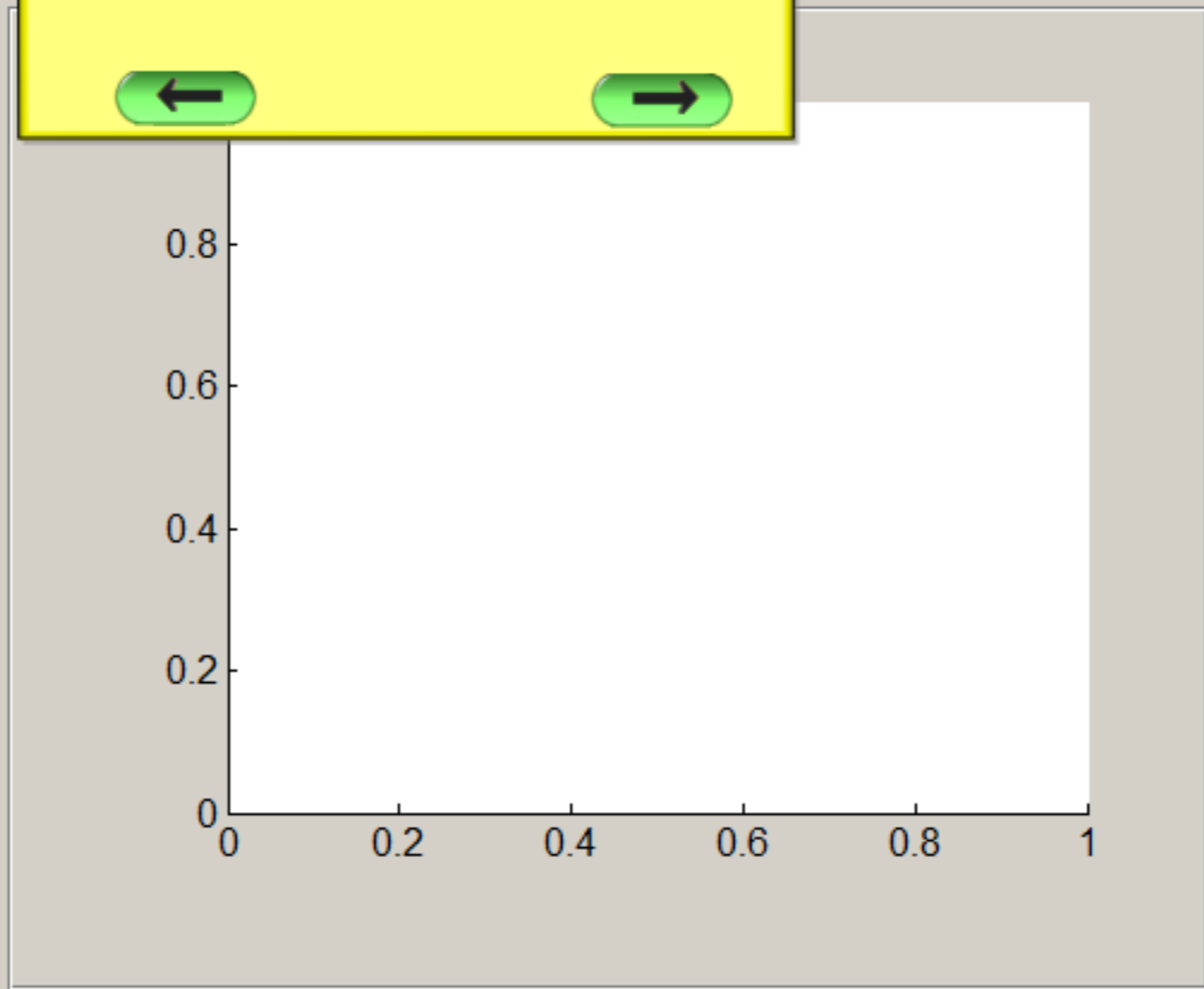
Choose an option below
None
Mean Center
Autoscale
Squareroot & mean center

Plot Scores and Loads

Select the pre processing method used on the data when you carried out PCA.

Peak List

- 285.2647--[M-H]C18
- 292.885--AuS3
- 333.2482--C18H37S
- 371.1106--AuMC10
- 393.9333--Au2
- 403.0822--AuS2C10f
- 425.9052--Au2S
- 457.8771--Au2S2
- 483.2357--AuMC18
- 489.8492--Au2S3
- 515.2086--Au[M-H]2C
- 543.2399--Au[M-H]2C



Select Plot Type

Average + Stdev Colored

Plot Peak Area Image

This plot will show the scaled for the selected peak after subtracting the PCs selected above.

Save Figure

Make Ext

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:

Load Selected Data

Image: **ndatassp**
Variable: **exactmass**
Scores: **scores**
Loads: **loads**

Data Preprocessing

PC #

Choose one:
Choose one:

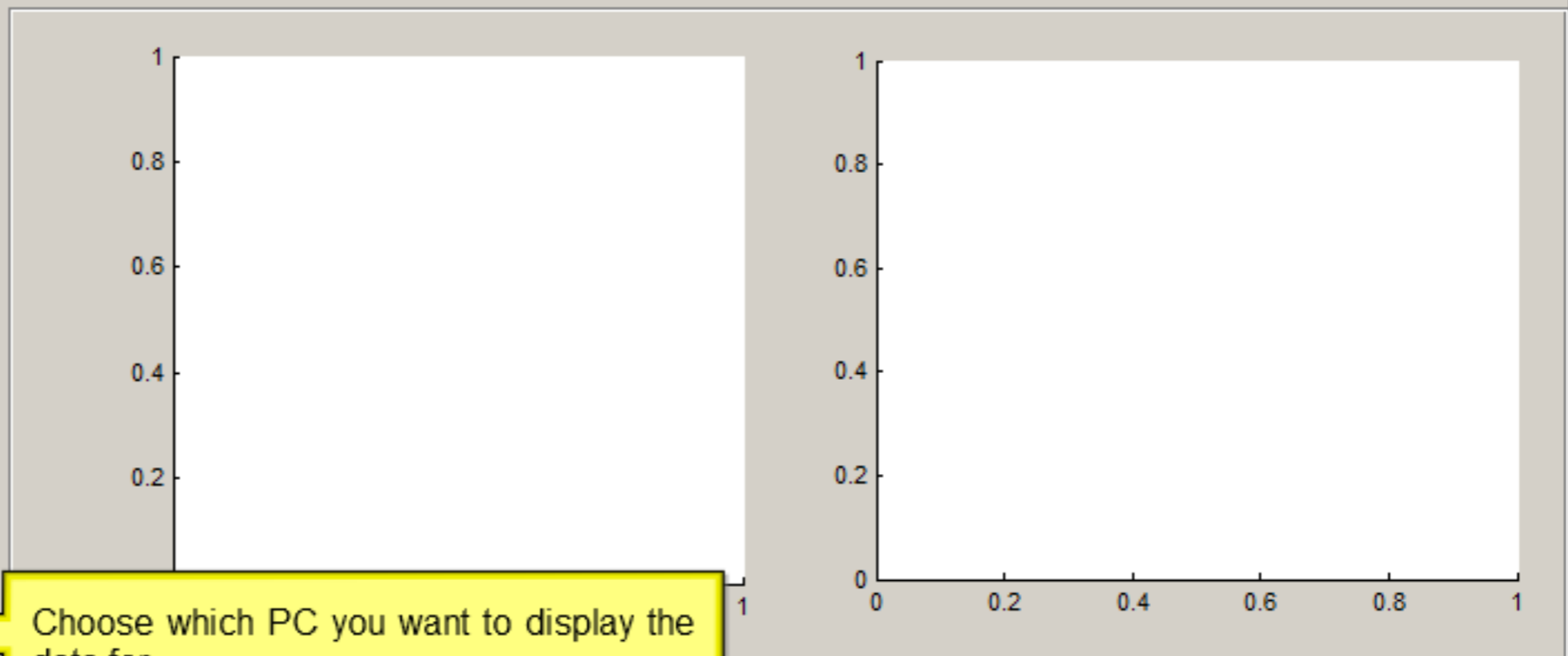
Peak List

- 285.2647--[M-H]C18
- 292.885--AuS3
- 333.2482--C18H37S
- 371.1106--AuMC10
- 393.9333--Au2
- 403.0822--AuS2C10
- 425.9052--Au2S
- 457.8771--Au2S2
- 483.2357--AuMC18
- 489.8492--Au2S3
- 515.2086--Au[M-H]2C
- 543.2399--Au[M-H]2C

Select Plot Type

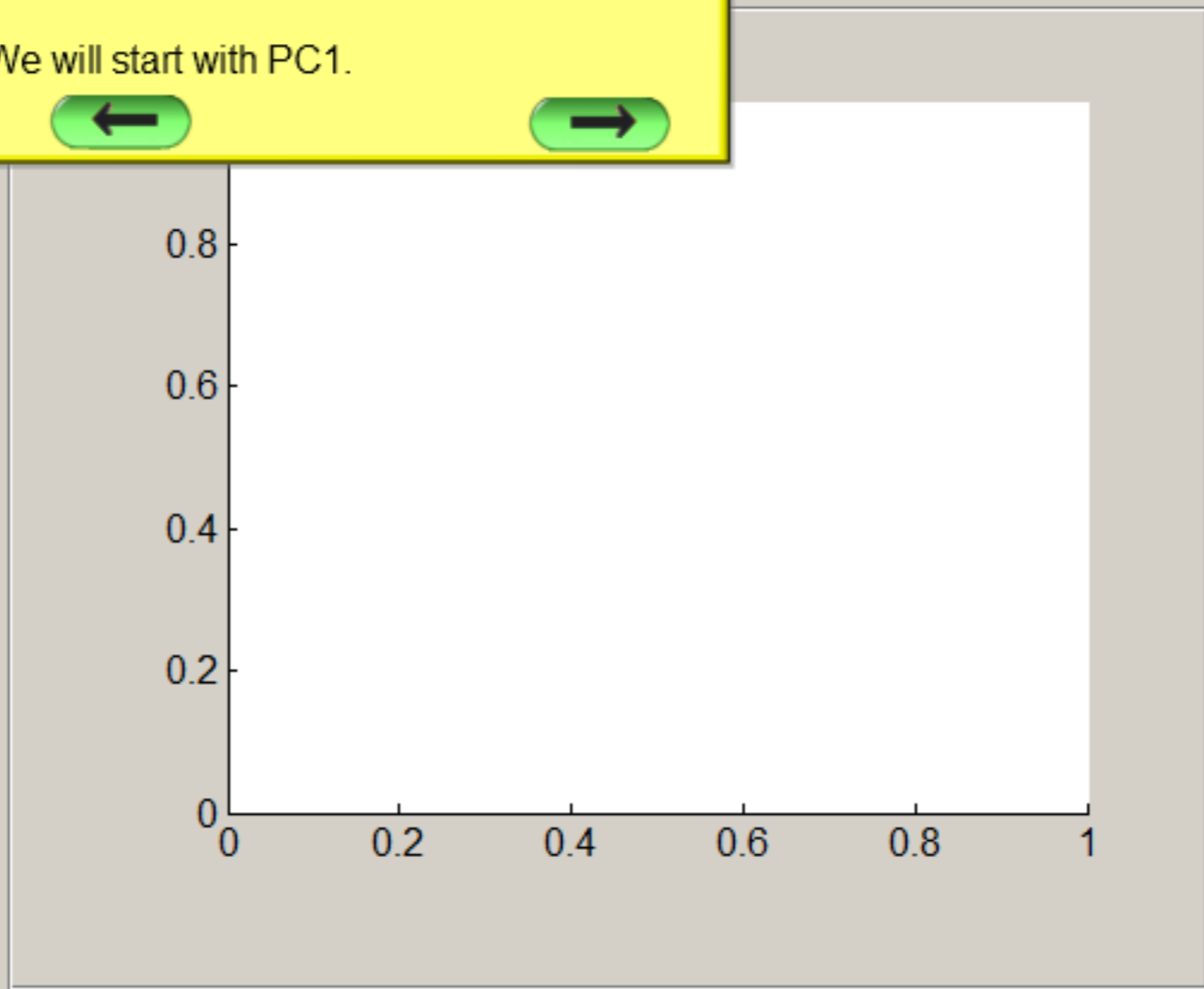
Plot Peak Area Image

This plot will show the scaled for the selected peak after subtracting the PCs selected above.



Choose which PC you want to display the data for.
We will start with PC1.

← →



Save Figure

Make Ext

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:

Load Selected Data

Image: **ndatassp**
 Variable: **exactmass**
 Scores: **scores**
 Loads: **loads**

Data Preprocessing

PC #

Plot Scores and Loads

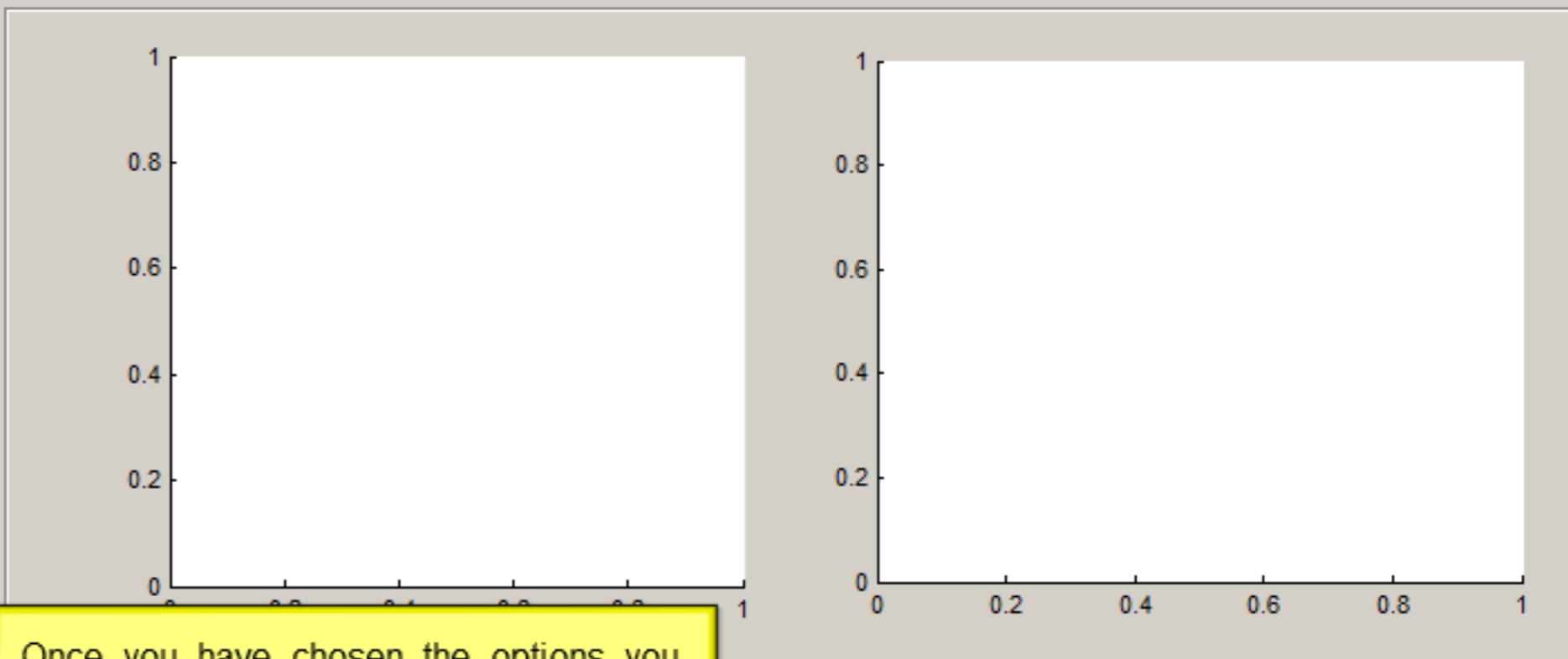
Peak List

- 285.2647--[M-H]C18
- 292.885--AuS3
- 333.2482--C18H37S
- 371.1106--AuMC10
- 393.9333--Au2
- 403.0822--AuS2C10
- 425.9052--Au2S
- 457.8771--Au2S2
- 483.2357--AuMC18
- 489.8492--Au2S3
- 515.2086--Au[M-H]2
- 543.2399--Au[M-H]2

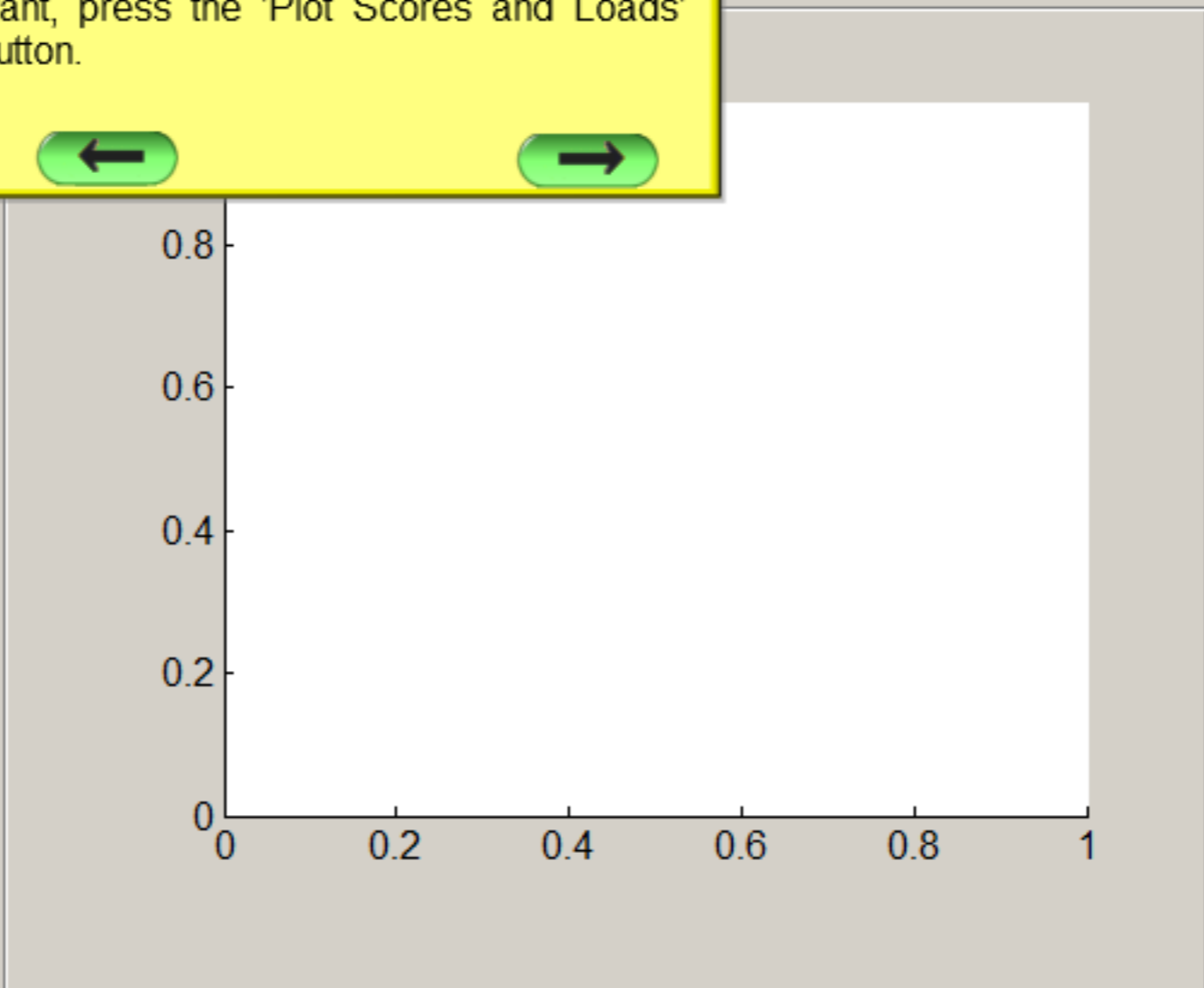
Select Plot Type

Plot Peak Area Image

This plot will show the scaled for the selected peak after subtracting the PCs selected above.



Once you have chosen the options you want, press the 'Plot Scores and Loads' button.



Save Figure

Make Ext

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:

Load Selected Data

Image: **ndatassp**
 Variable: **exactmass**
 Scores: **scores**
 Loads: **loads**

Data Preprocessing

PC #

Plot Scores and Loads

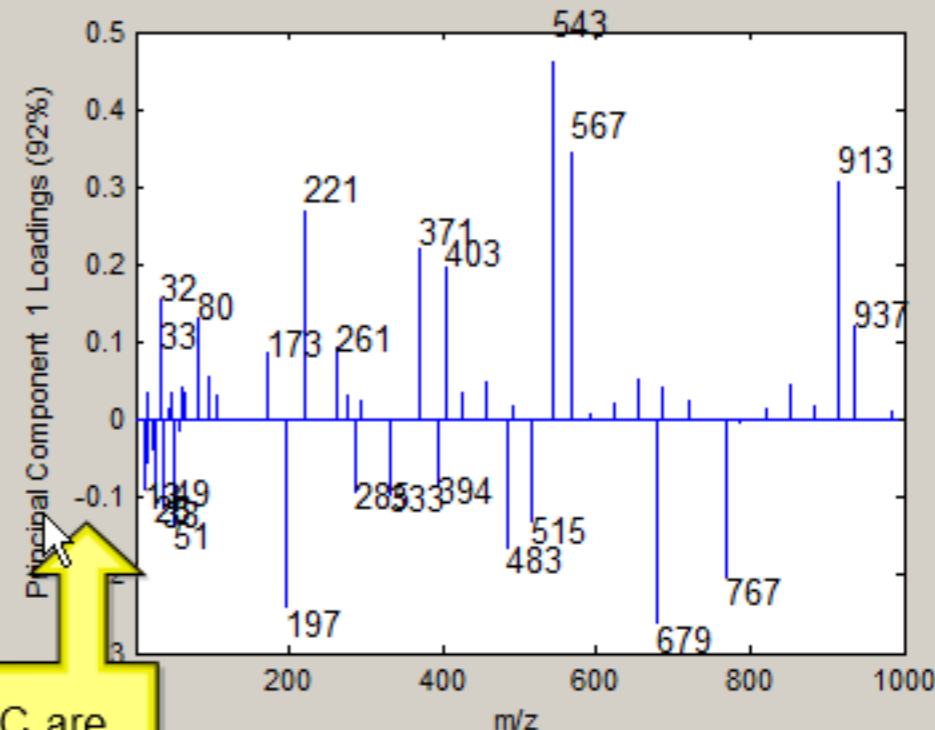
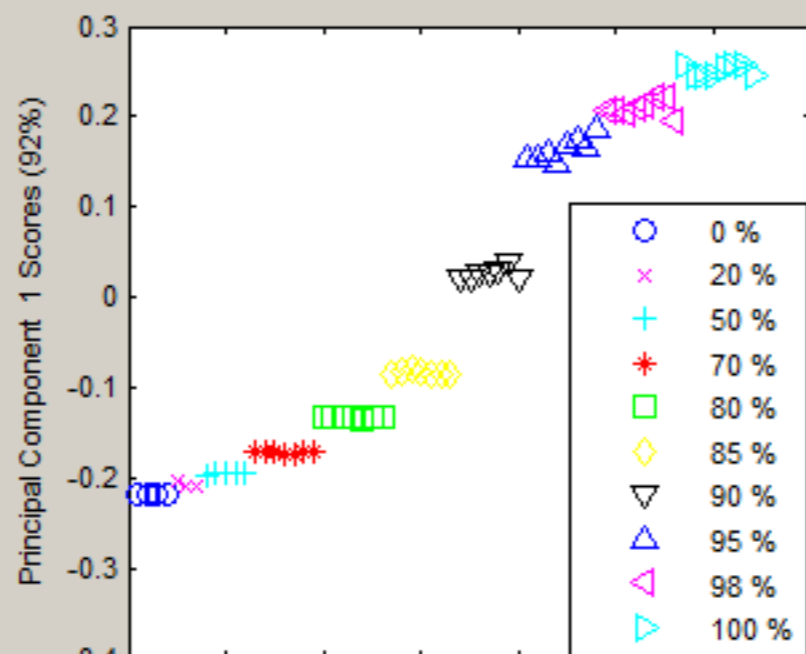
Peak List

- 285.2647--[M-H]C18
- 292.885--AuS3
- 333.2482--C18H37S
- 371.1106--AuMC10
- 393.9333--Au2
- 403.0822--AuS2C10
- 425.9052--Au2S
- 457.8771--Au2S2
- 483.2357--AuMC18
- 489.8492--Au2S3
- 515.2086--Au[M-H]2
- 543.2399--Au[M-H]2

Select Plot Type

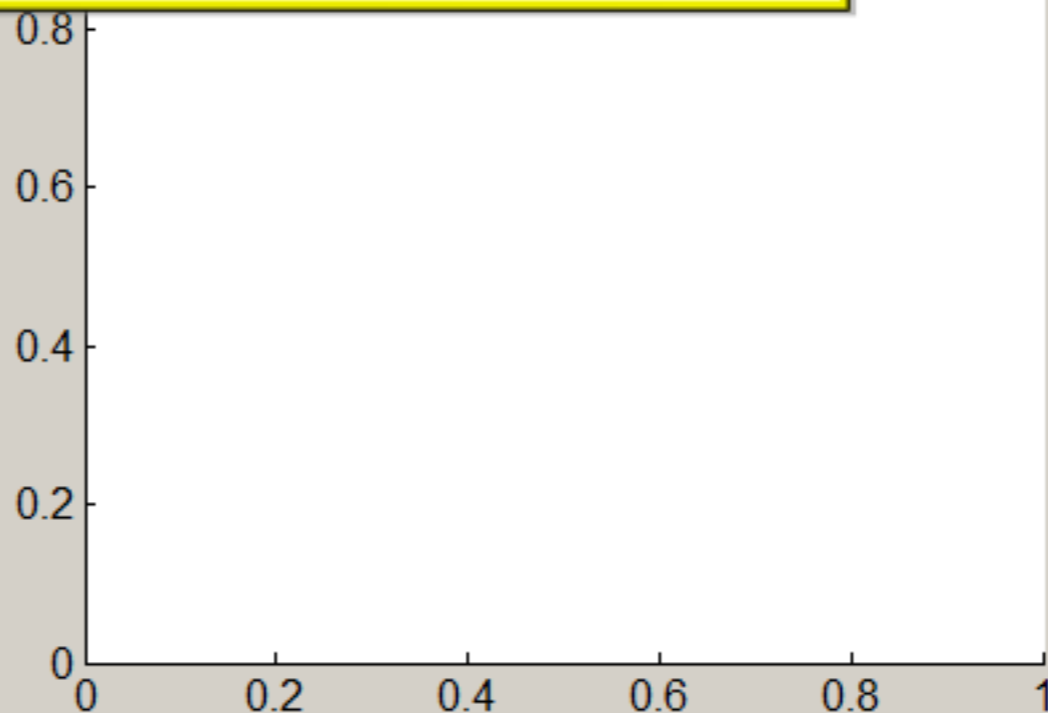
Plot Peak Area Image

This plot will show the scaled for the selected peak after subtracting the PCs selected above.



The scores and loadings for the chosen PC are displayed.

Here we can see that the peak at m/z 543 has a high positive loading on PC1.



Save Figure

Make Ext

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:

Load Selected Data

Image: **ndatassp**
Variable: **exactmass**
Scores: **scores**
Loads: **loads**

Data Preprocessing

PC #

Plot Scores and Loads

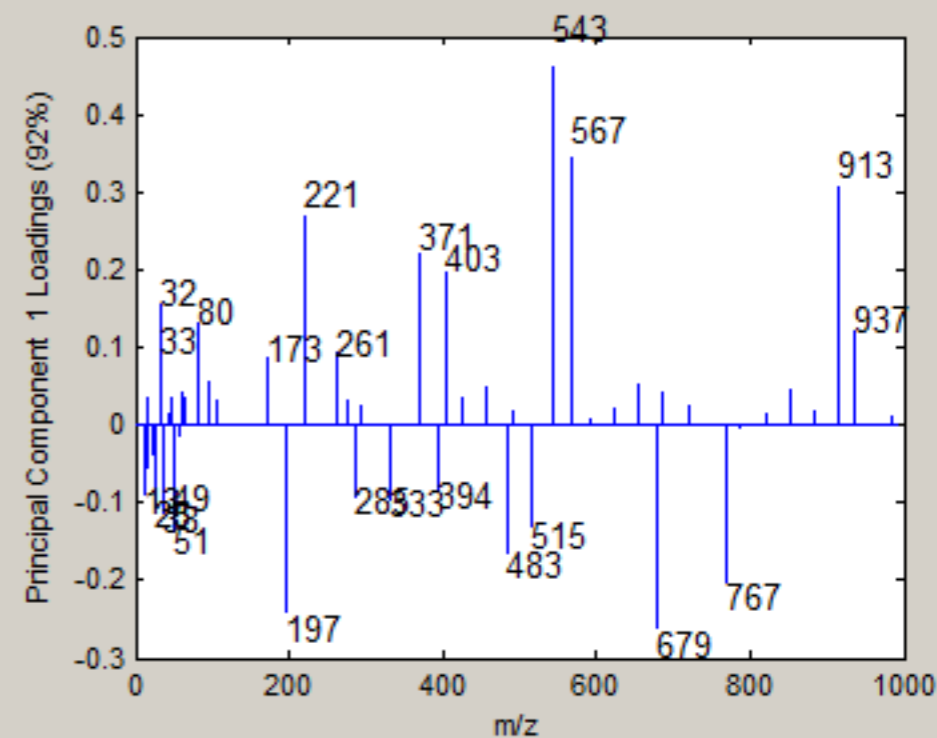
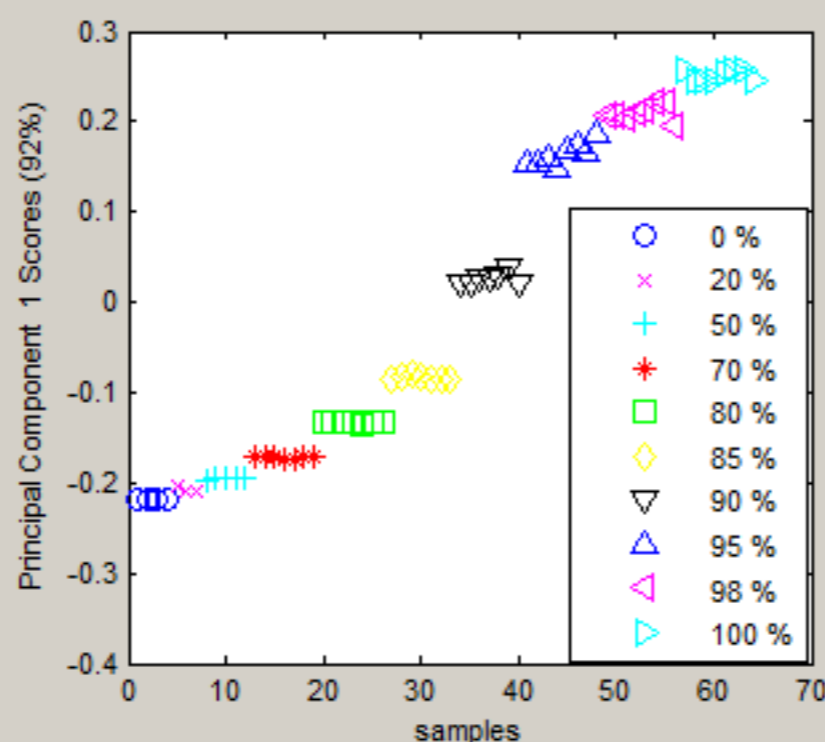
Peak List

- 333.2482--C18H37S
- 371.1106--AuMC10
- 393.9333--Au2
- 403.0822--AuS2C10f
- 425.9052--Au2S
- 457.8771--Au2S2
- 483.2357--AuMC18
- 489.8492--Au2S3
- 515.2086--Au[M-H]2
- 543.2399--Au[M-H]2**
- 567.0683--Au2[M-H]c
- 590.8999--Au3

Select Plot Type

Plot Peak Area Image

This plot will show the scaled for the selected peak after subtracting the PCs selected above.



Let's select the m/z 543 peak.



Save Figure

Make Ext

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:

Load Selected Data

Image: **ndatassp**
 Variable: **exactmass**
 Scores: **scores**
 Loads: **loads**

Data Preprocessing

PC #

Plot Scores and Loads

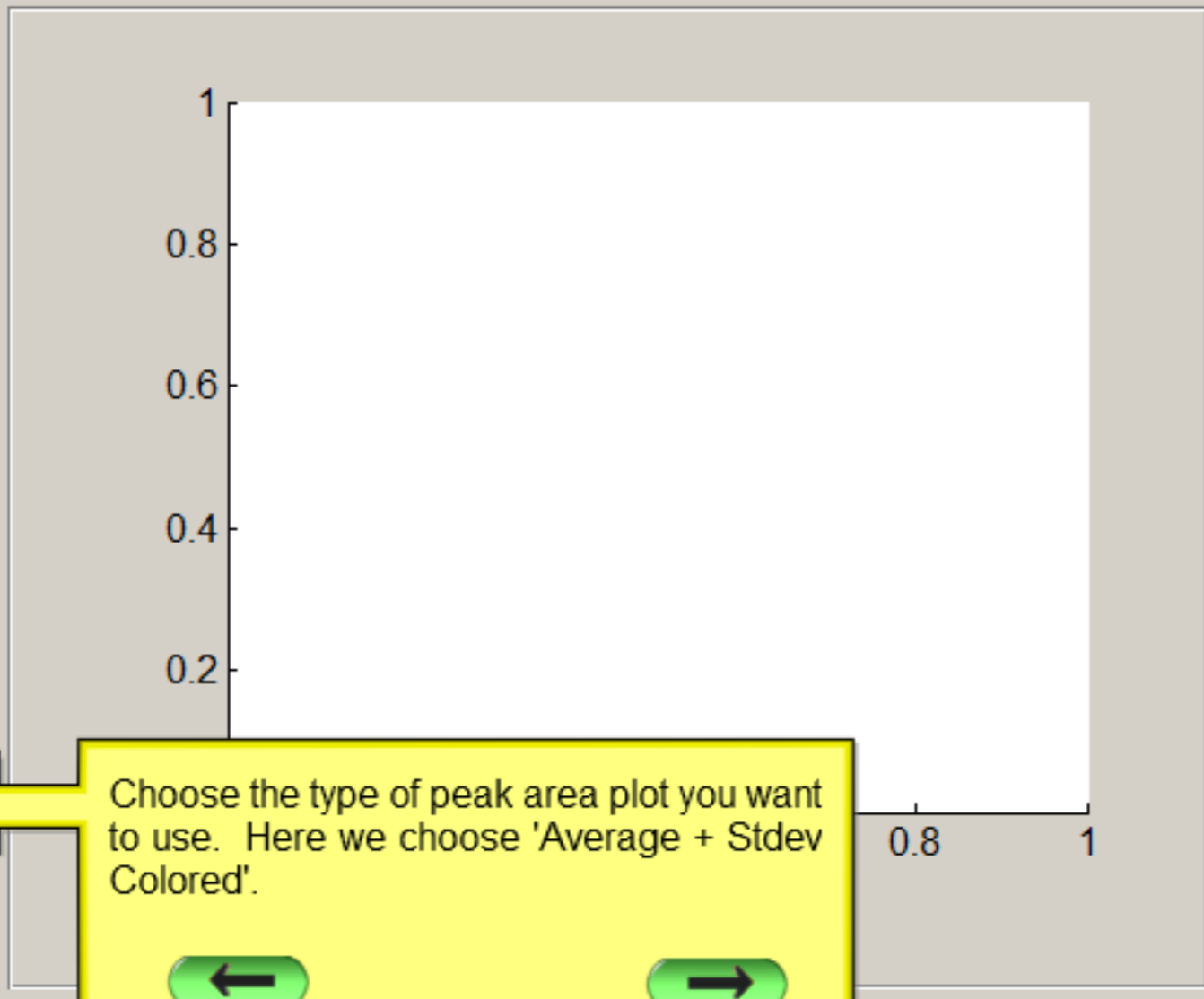
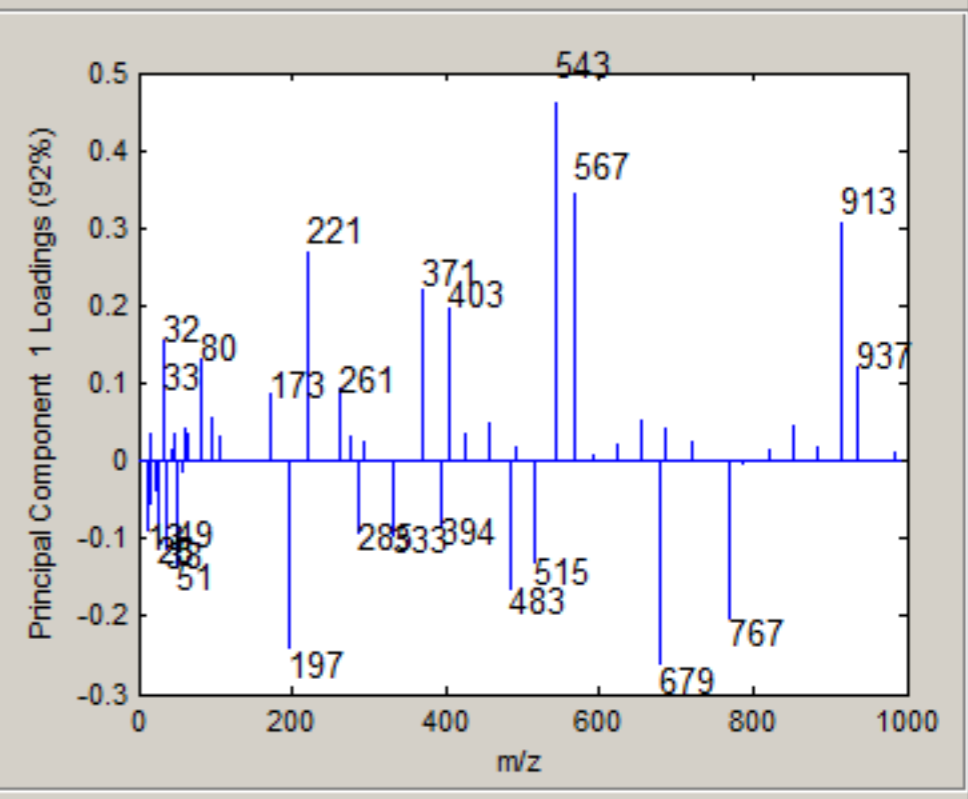
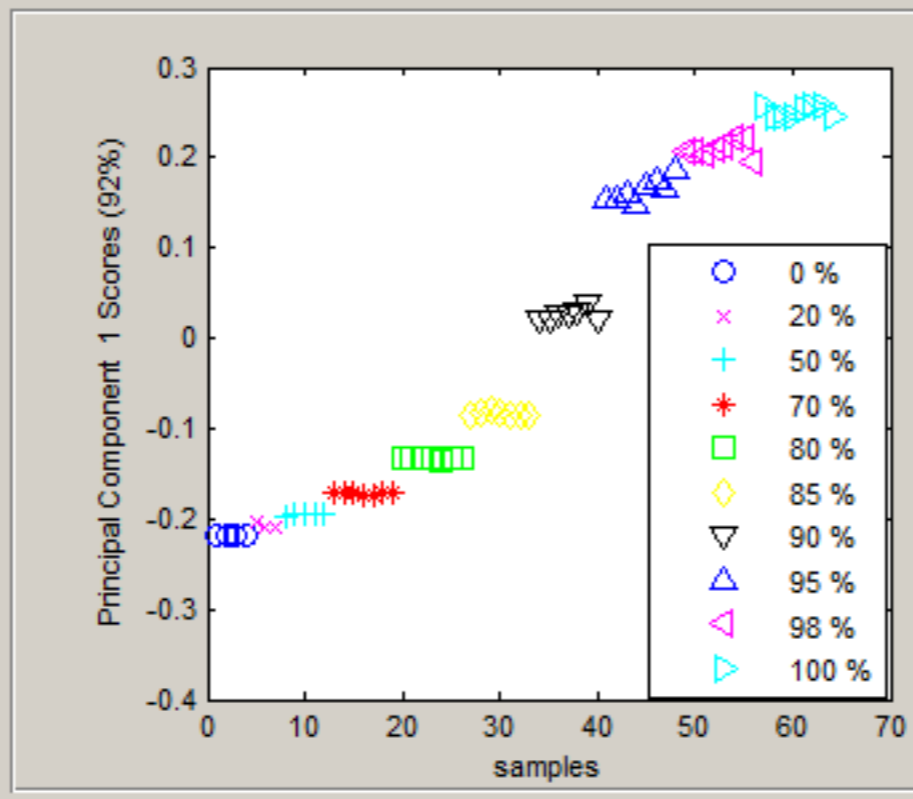
Peak List

- 333.2482--C18H37S
- 371.1106--AuMC10
- 393.9333--Au2
- 403.0822--AuS2C10f
- 425.9052--Au2S
- 457.8771--Au2S2
- 483.2357--AuMC18
- 489.8492--Au2S3
- 515.2086--Au[M-H]20
- 543.2399--Au[M-H]20
- 567.0683--Au2[M-H]0
- 590.8999--Au3

Select Plot Type

Choose Plot Style

- Scatter
- Bar
- Average + Stdev
- Average + Stdev Colored**



Save Figure

Make Ext

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:

Load Selected Data

Image: **ndatassp**
 Variable: **exactmass**
 Scores: **scores**
 Loads: **loads**

Data Preprocessing

PC #

Plot Scores and Loads

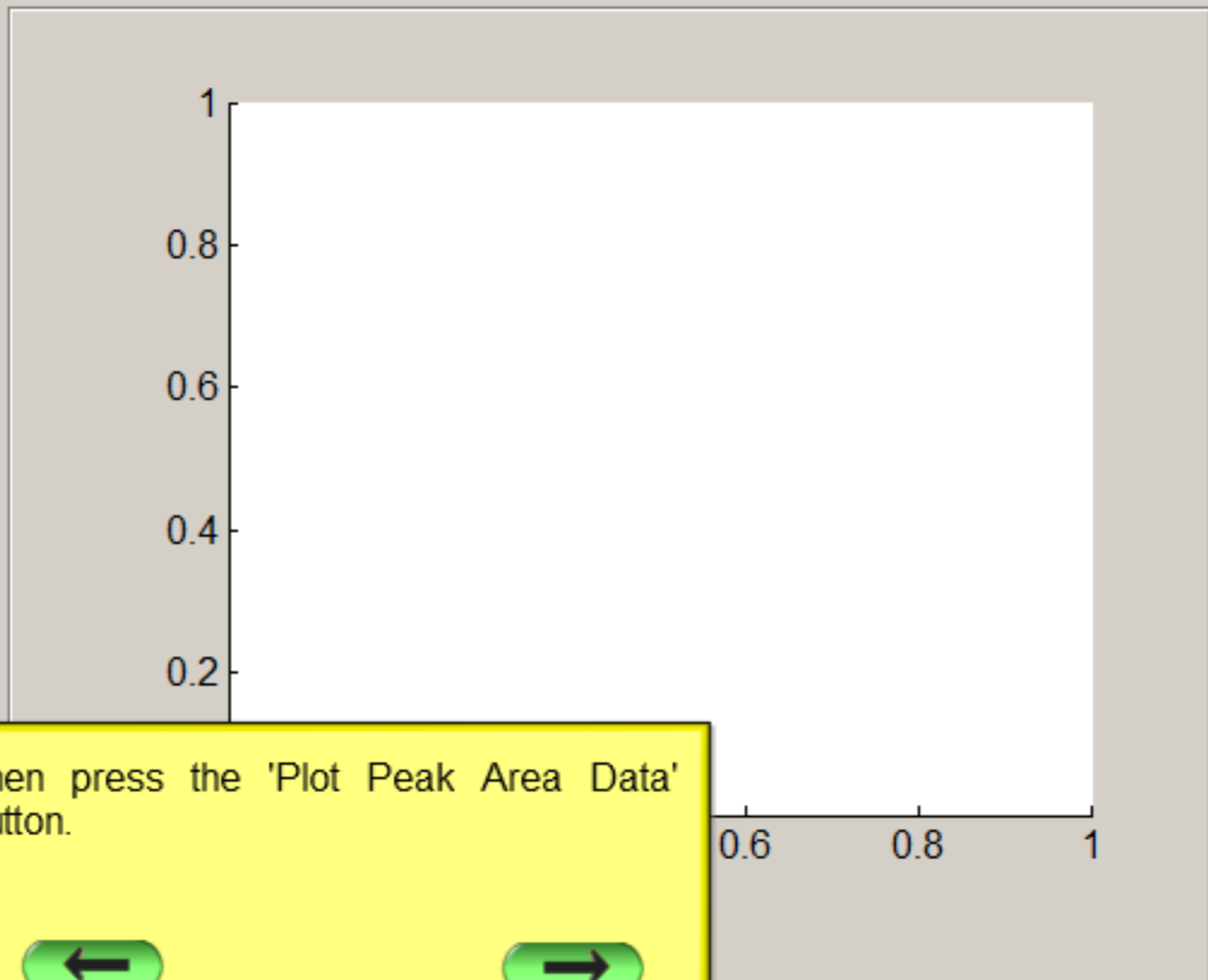
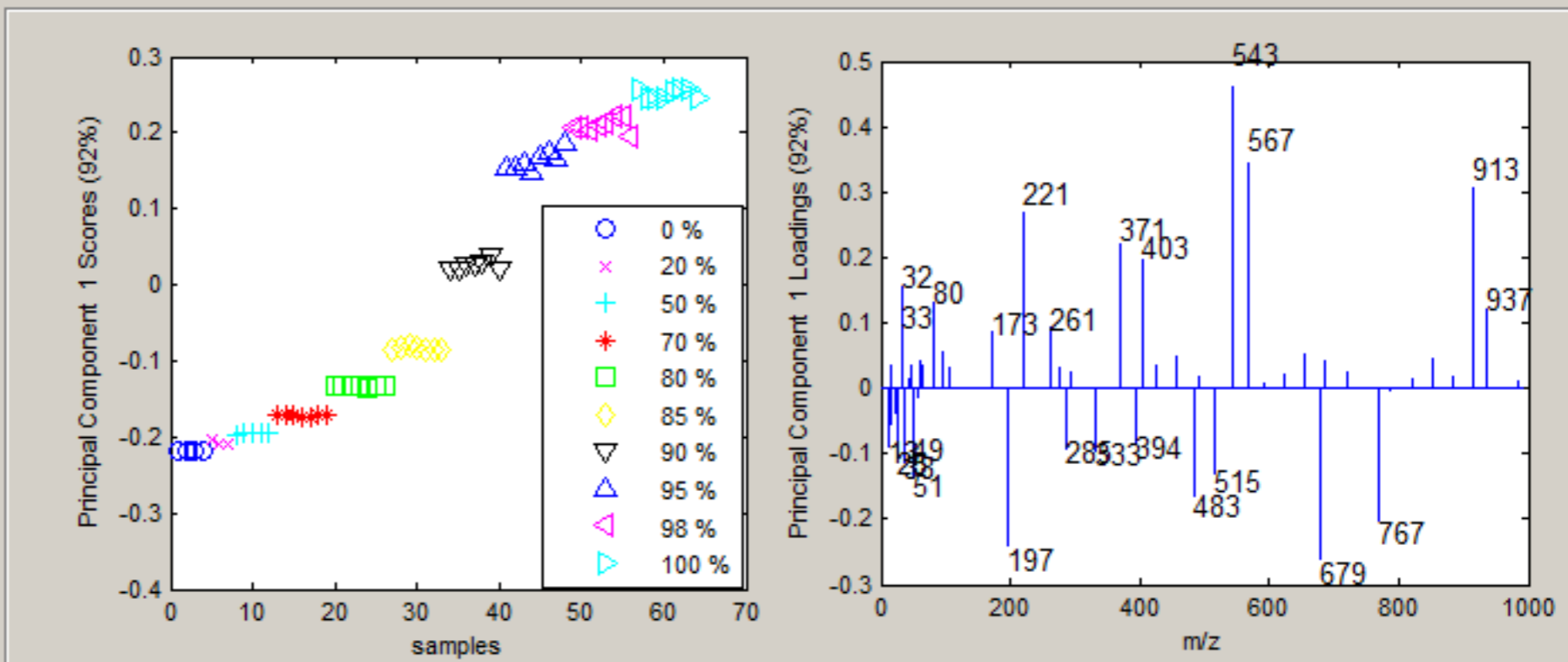
Peak List

- 333.2482--C18H37S
- 371.1106--AuMC10
- 393.9333--Au2
- 403.0822--AuS2C10f
- 425.9052--Au2S
- 457.8771--Au2S2
- 483.2357--AuMC18
- 489.8492--Au2S3
- 515.2086--Au[M-H]20
- 543.2399--Au[M-H]20
- 567.0683--Au2[M-H]0
- 590.8999--Au3

Select Plot Type

Plot Peak Area Image

This plot will show the scaled for the selected peak after subtracting the PCs selected above.



Save Figure

Make Ext

Close Panel

Then press the 'Plot Peak Area Data' 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:
 Name of Variable Matrix:
 Name of Filename Matrix:
 Name of Totalcounts Matrix:
 Name of Samplenames Matrix:

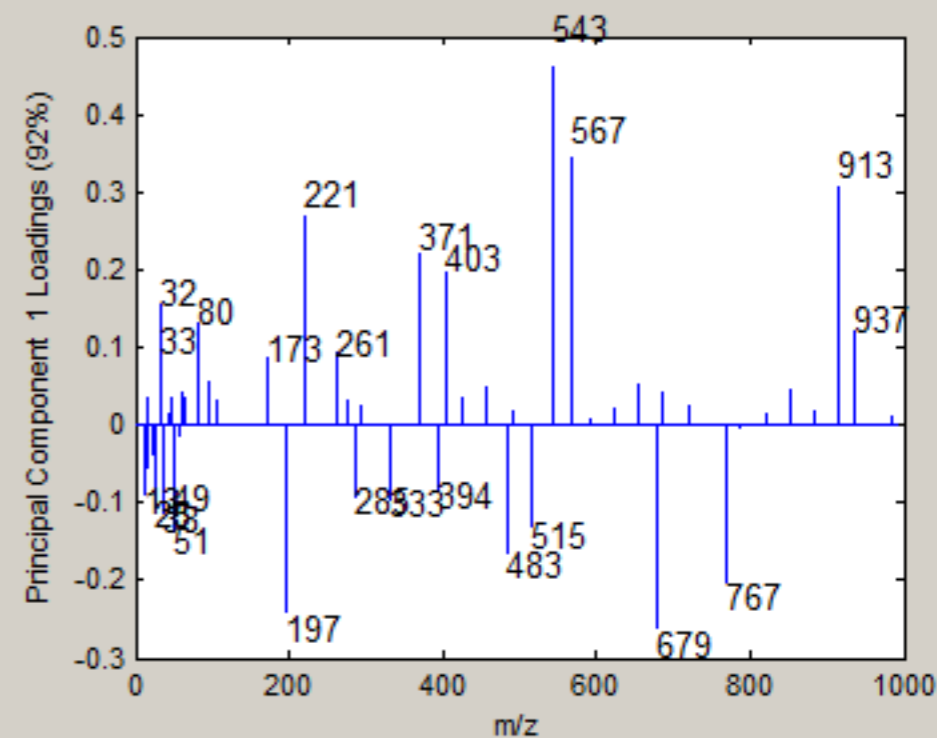
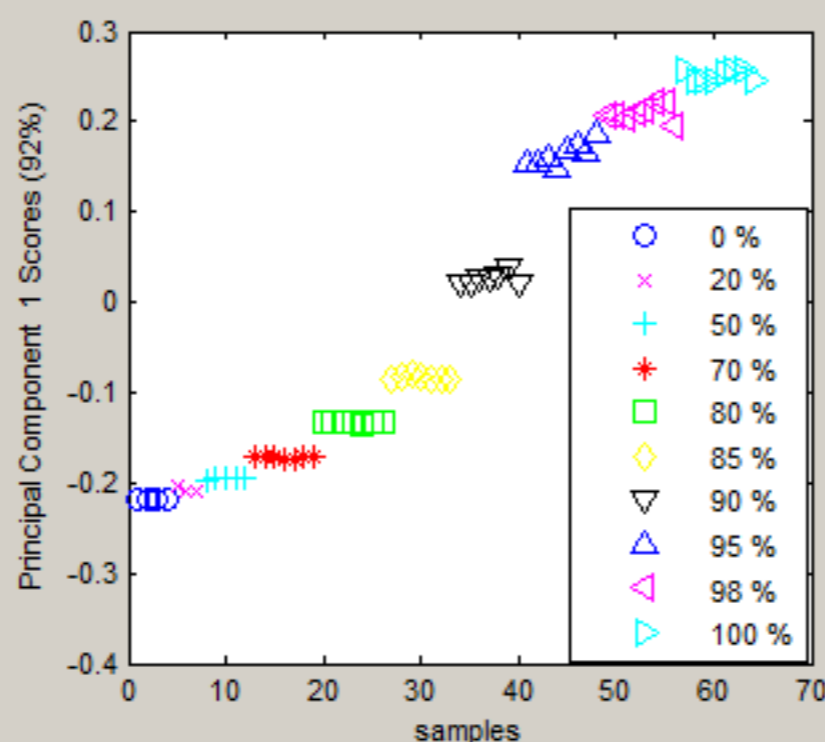
Load Selected Data

Image: **ndatassp**
 Variable: **exactmass**
 Scores: **scores**
 Loads: **loads**

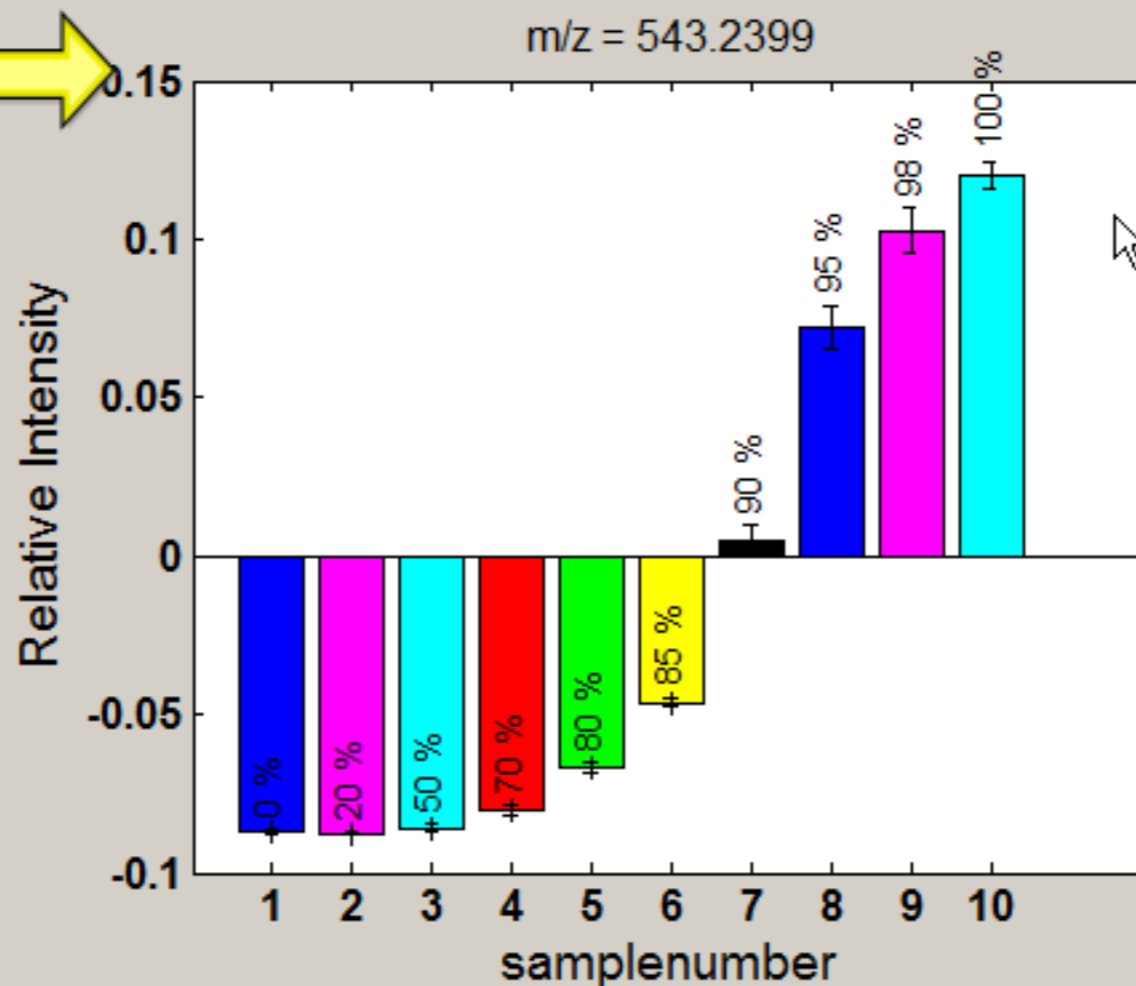
Data Preprocessing

PC #

Plot Scores and Loads



Here we see the pre processed peak area data for the m/z 543 peak. It looks very similar to the PC1 scores image as we would expect since this peak has a high positive loading on this PC and therefore we would expect it to have a higher relative intensity in areas with positive scores on PC1.



Save Figure

Make Ext

Close Panel

590.8999--Au3

Select Plot Type

Plot Peak Area Image

This plot will show the scaled for the selected peak after subtracting the PCs selected above.

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:

Load Selected Data

Image: **ndatassp**
 Variable: **exactmass**
 Scores: **scores**
 Loads: **loads**

Data Preprocessing

PC #

Choose one:

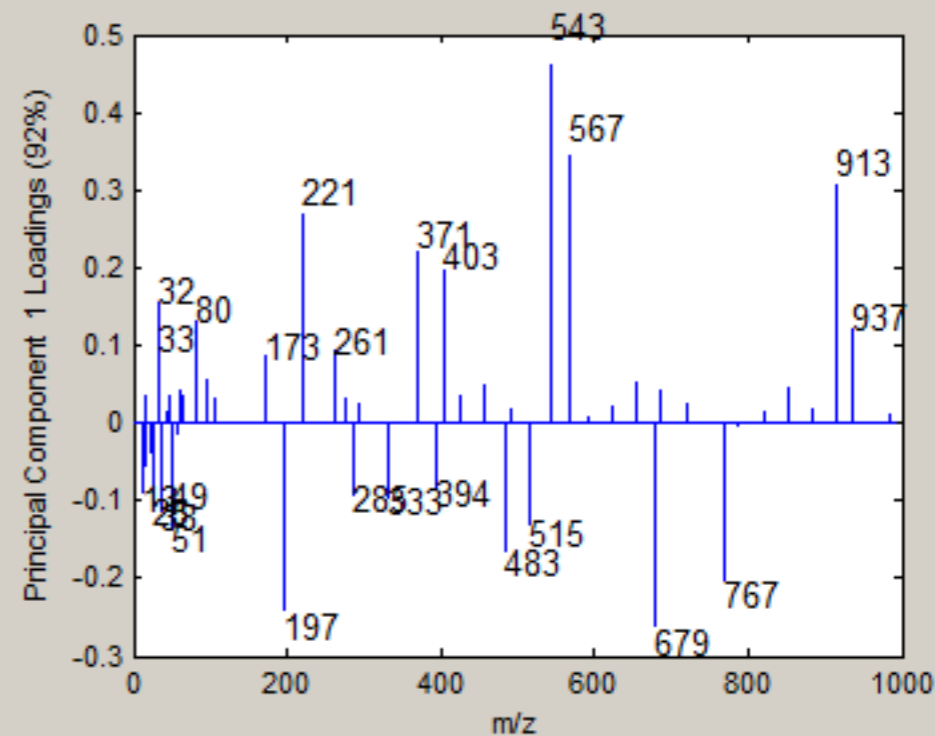
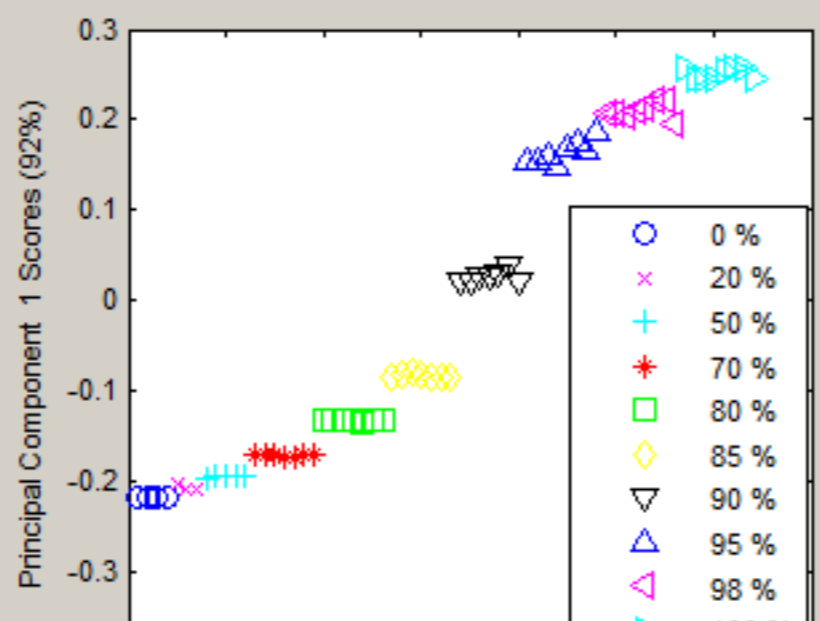
Peak List

- 333.2482--C18H37S
- 371.1106--AuMC10
- 393.9333--Au2
- 403.0822--AuS2C10f
- 425.9052--Au2S
- 457.8771--Au2S2
- 483.2357--AuMC18
- 489.8492--Au2S3
- 515.2086--Au[M-H]2
- 543.2399--Au[M-H]2
- 567.0683--Au2[M-H]C
- 590.8999--Au3

Select Plot Type

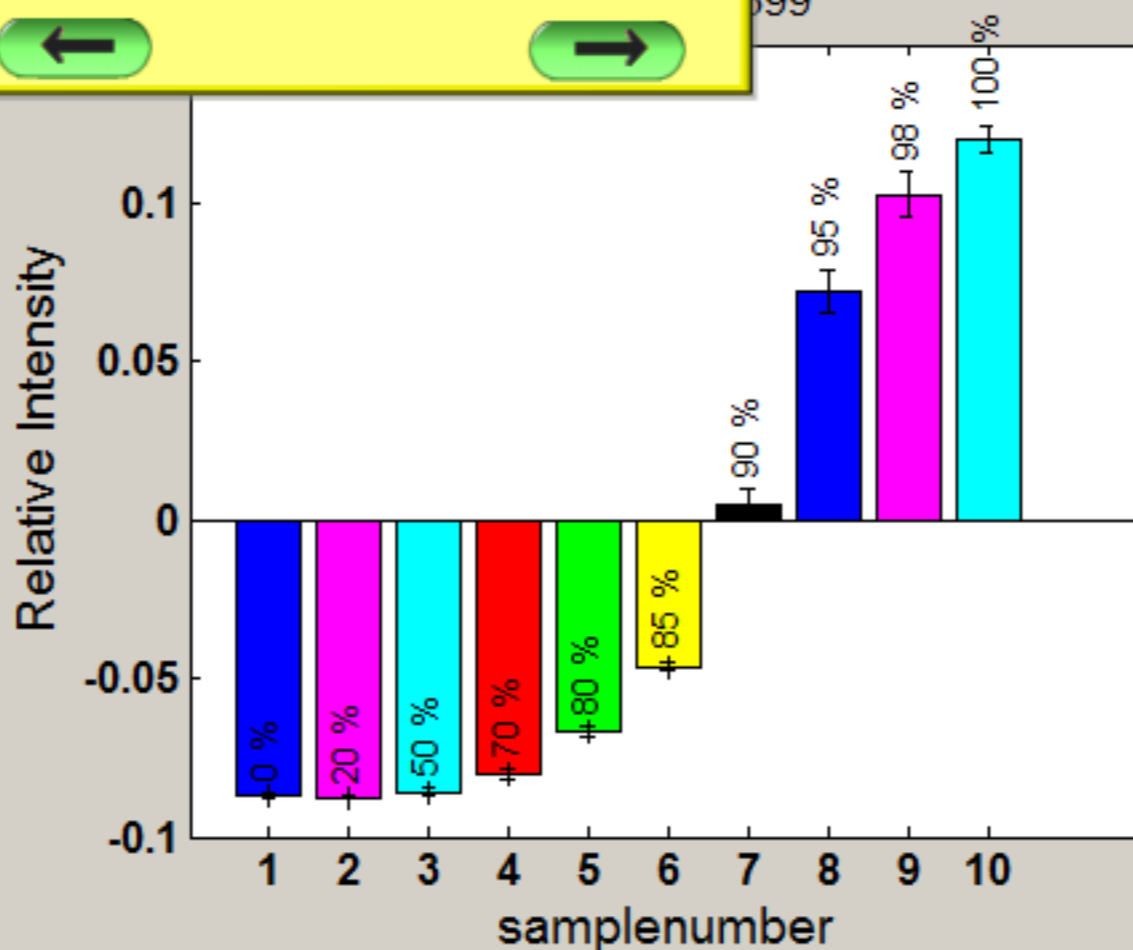
Plot Peak Area Image

This plot will show the scaled for the selected peak after subtracting the PCs selected above.



Now lets look at PC2 by selecting it from the drop down menu.

← →



Save Figure

Make Ext

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:

Load Selected Data

Image: **ndatassp**
 Variable: **exactmass**
 Scores: **scores**
 Loads: **loads**

Data Preprocessing

PC #

Plot Scores and Loads

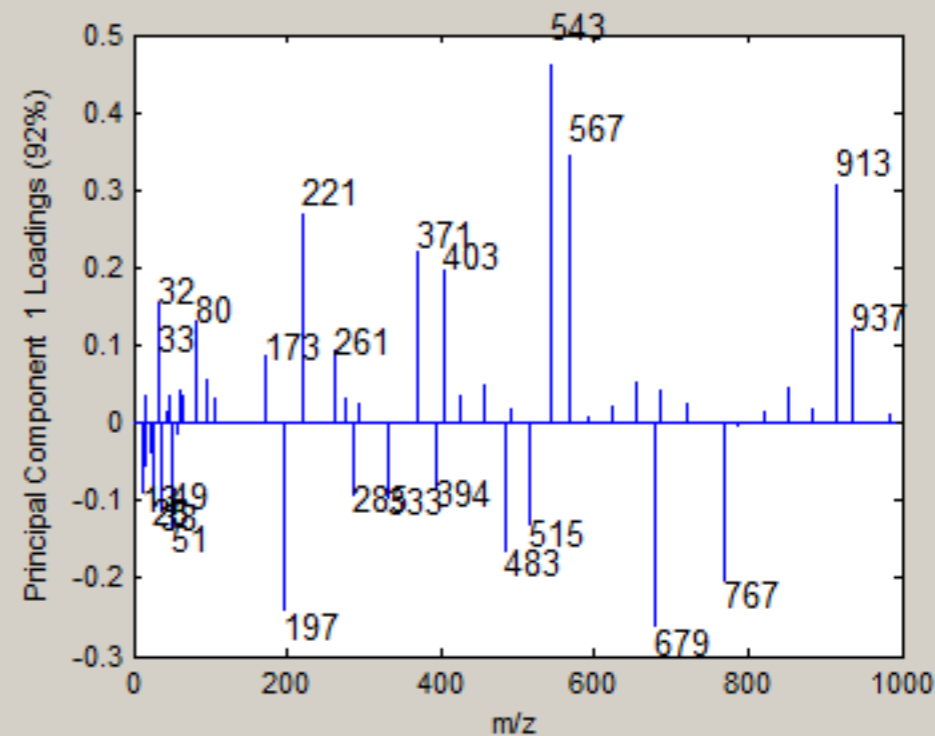
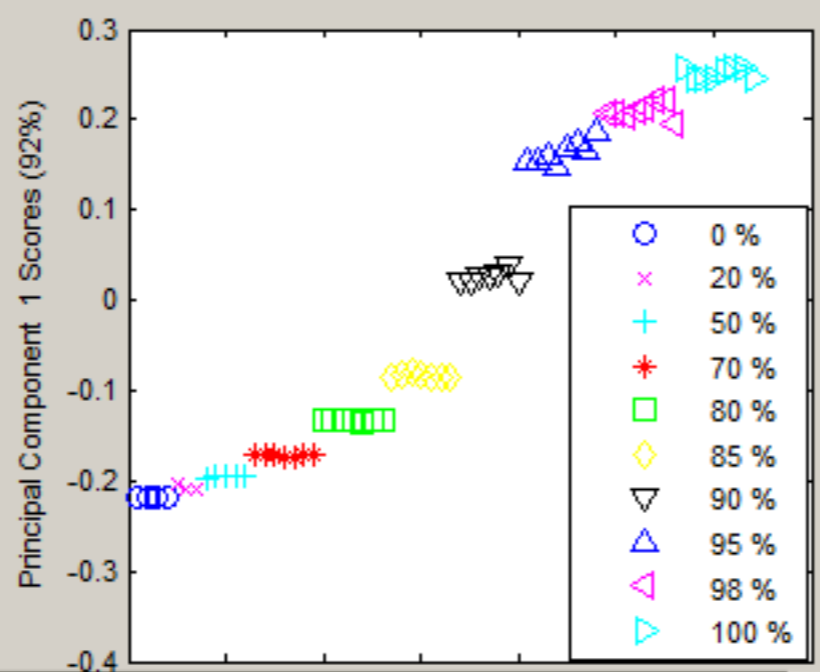
Peak List

- 333.2482--C18H37S
- 371.1106--AuMC10
- 393.9333--Au2
- 403.0822--AuS2C10f
- 425.9052--Au2S
- 457.8771--Au2S2
- 483.2357--AuMC18
- 489.8492--Au2S3
- 515.2086--Au[M-H]2
- 543.2399--Au[M-H]2
- 567.0683--Au2[M-H]C
- 590.8999--Au3

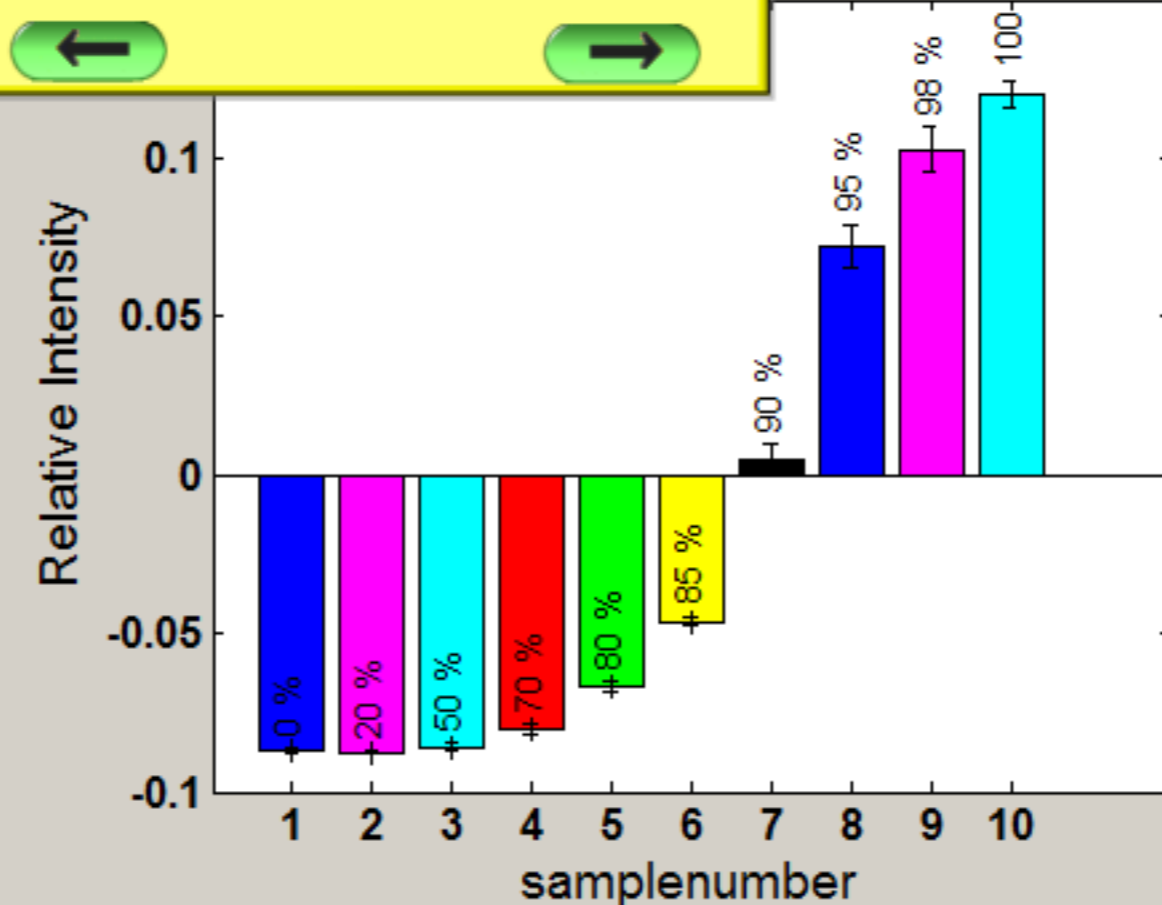
Select Plot Type

Plot Peak Area Image

This plot will show the scaled for the selected peak after subtracting the PCs selected above.



And pressing the 'Plot Scores and Loads' button.



Save Figure

Make Ext

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:

Load Selected Data

Image: **ndatassp**
 Variable: **exactmass**
 Scores: **scores**
 Loads: **loads**

Data Preprocessing

PC #

Plot Scores and Loads

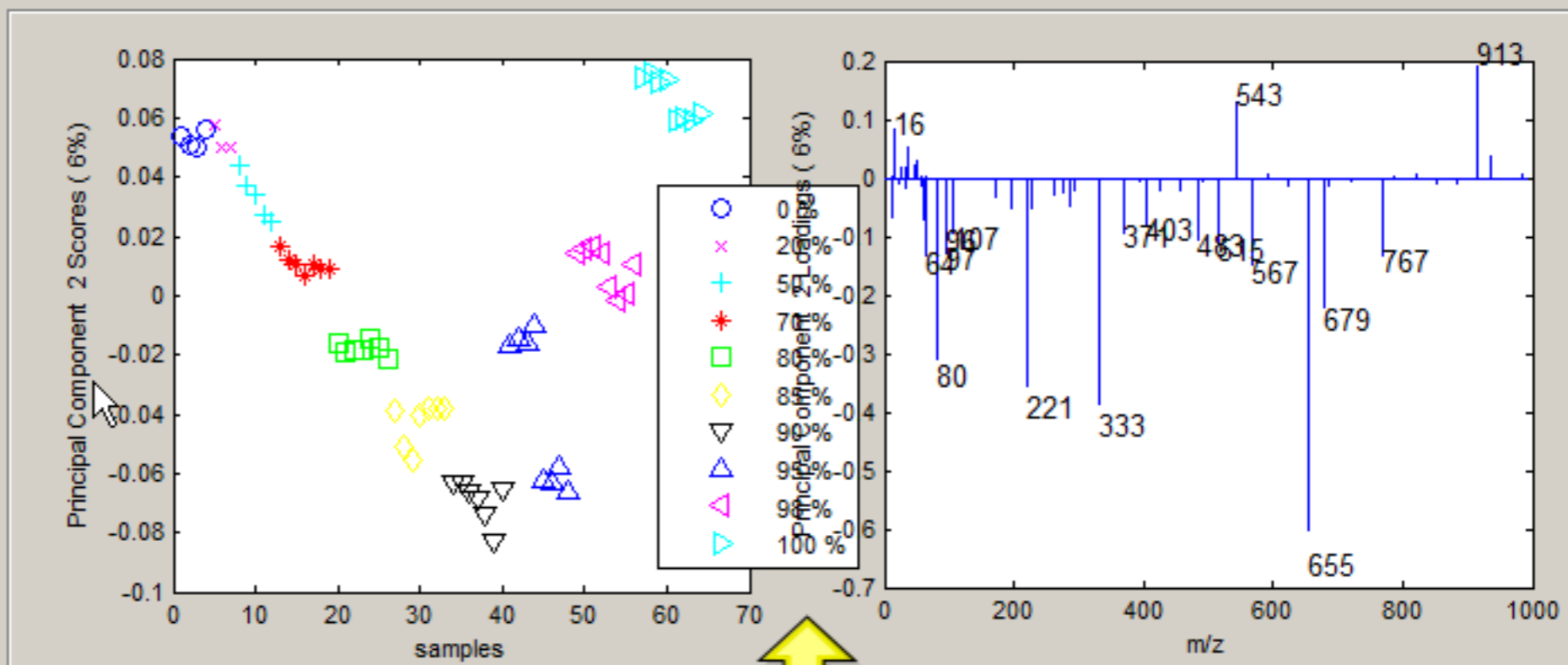
Peak List

- 333.2482--C18H37S
- 371.1106--AuMC10
- 393.9333--Au2
- 403.0822--AuS2C10f
- 425.9052--Au2S
- 457.8771--Au2S2
- 483.2357--AuMC18
- 489.8492--Au2S3
- 515.2086--Au[M-H]2
- 543.2399--Au[M-H]2
- 567.0683--Au2[M-H]C
- 590.8999--Au3

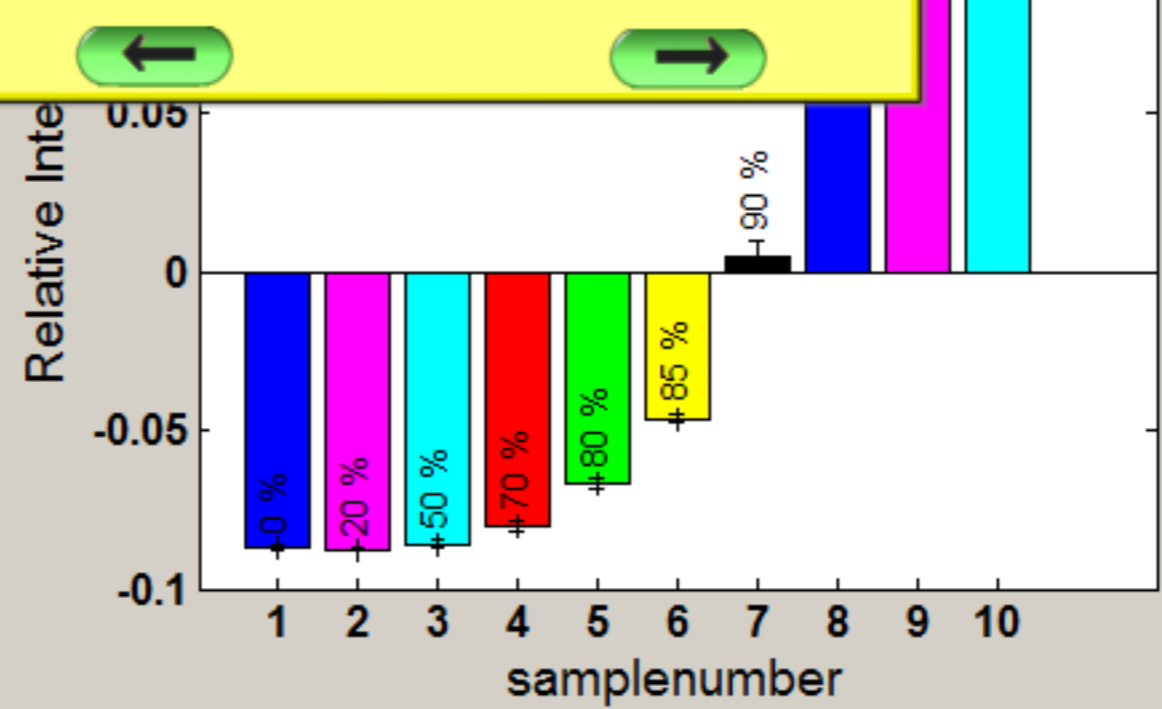
Select Plot Type

Plot Peak Area Image

This plot will show the scaled for the selected peak after subtracting the PCs selected above.



The PC2 scores show a different pattern than PC1. The m/z 543 peak shows a positive loading on PC2, but it no longer has the highest loading.



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:

Load Selected Data

Image: **ndatassp**
 Variable: **exactmass**
 Scores: **scores**
 Loads: **loads**

Data Preprocessing

PC #

Plot Scores and Loads

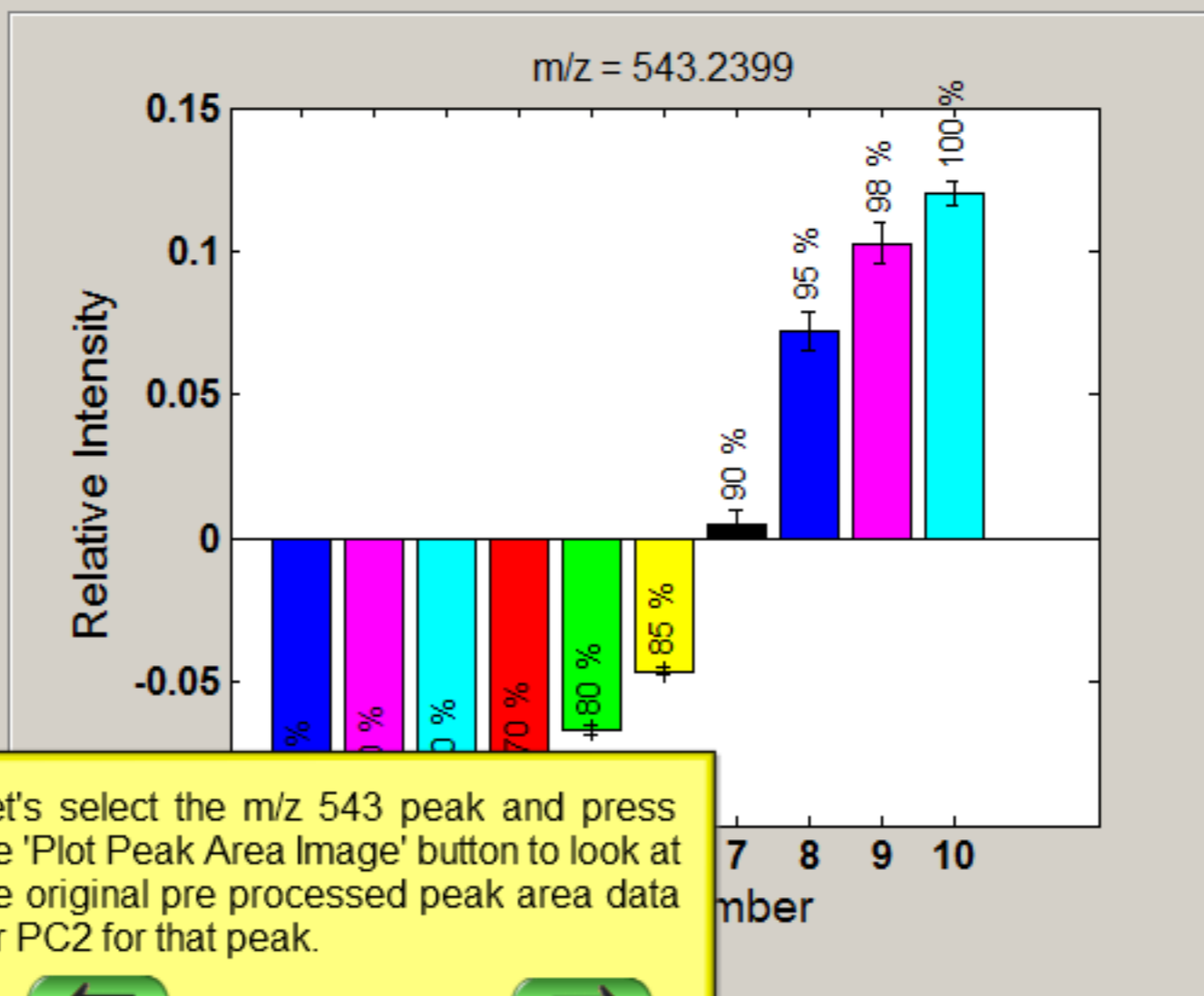
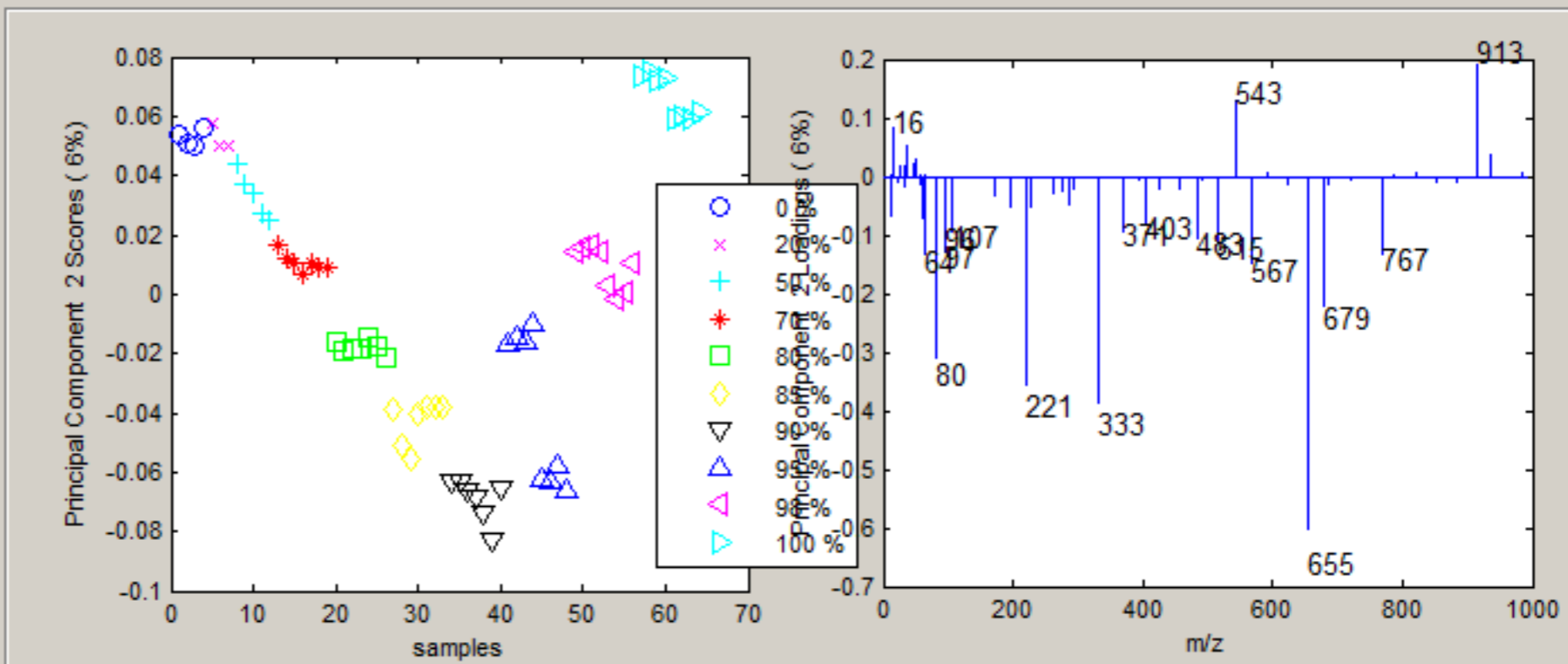
Peak List

- 333.2482--C18H37S
- 371.1106--AuMC10
- 393.9333--Au2
- 403.0822--AuS2C10f
- 425.9052--Au2S
- 457.8771--Au2S2
- 483.2357--AuMC18
- 489.8492--Au2S3
- 515.2086--Au[M-H]2
- 543.2399--Au[M-H]2
- 567.0683--Au2[M-H]C
- 590.8999--Au3

Select Plot Type

Plot Peak Area Image

This plot will show the scaled for the selected peak after subtracting the PCs selected above.



Save Figure

Make Ext

Close Panel

Let's select the m/z 543 peak and press the 'Plot Peak Area Image' button to look at the original pre processed peak area data for PC2 for that peak.

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.

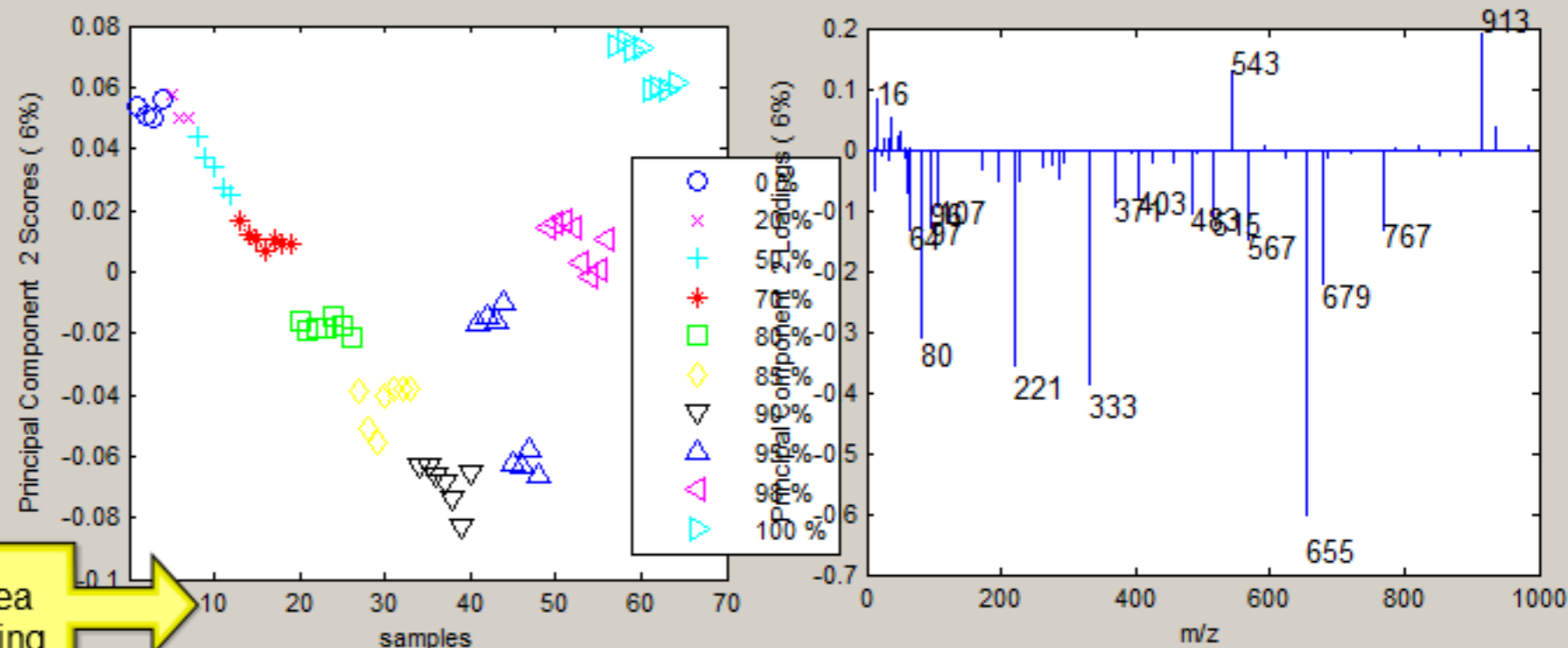
Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

Load Selected Data

Image: **ndatassp**
 Variable: **exactmass**
 Scores: **scores**
 Loads: **loads**

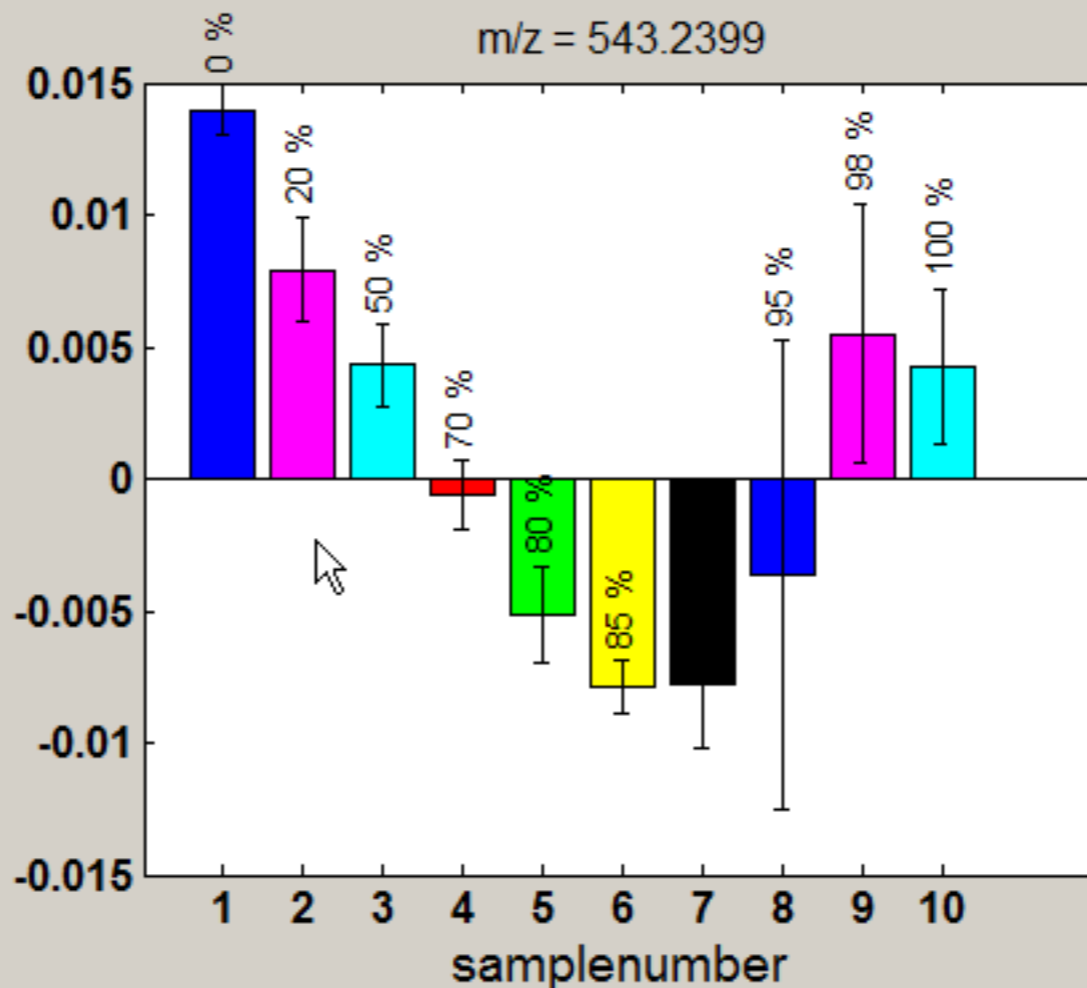
Data Preprocessing

PC #



Here we see the pre processed peak area data for the m/z 543 peak after subtracting PC1 from the data set. The general pattern is similar to that seen in the PC2 scores, and it is very different from that seen before subtracting PC1 from the data set.

This plot makes more sense than the plot from the pre processed data before subtracting PC1 for understanding what is happening in PC2. Before subtracting PC1 the m/z 543 peak area data showed an increase with increasing sample number. For PC2 the data shows a decrease and then an increase exactly like is seen in the scores plot.



Save Figure

Make Ext

Close Panel

This plot will show the scaled for the selected peak after subtracting the PCs selected above.

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.

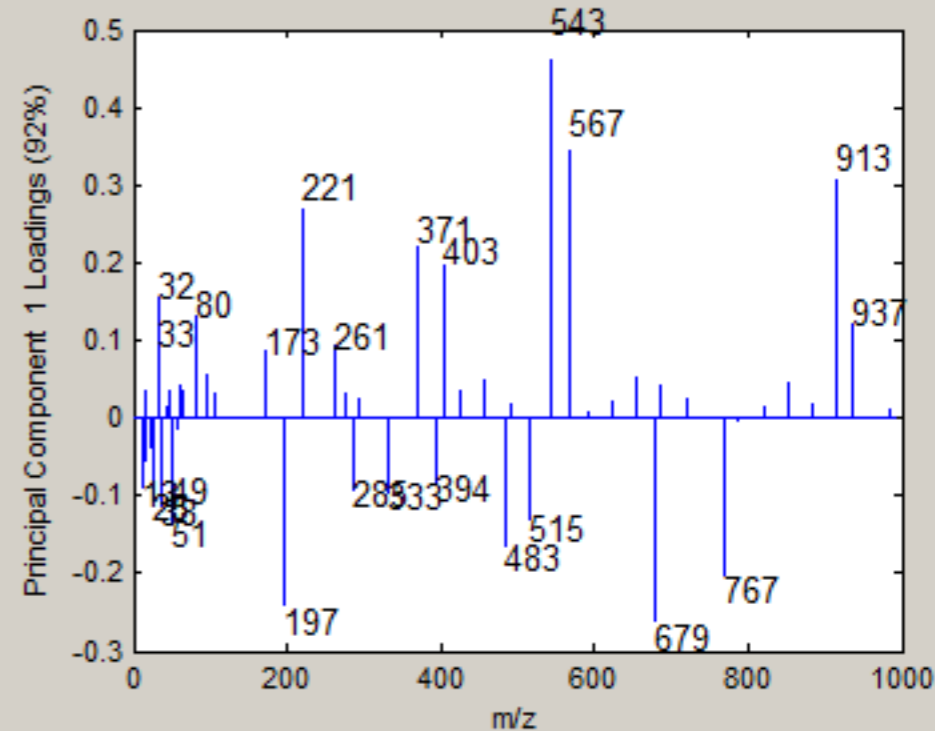
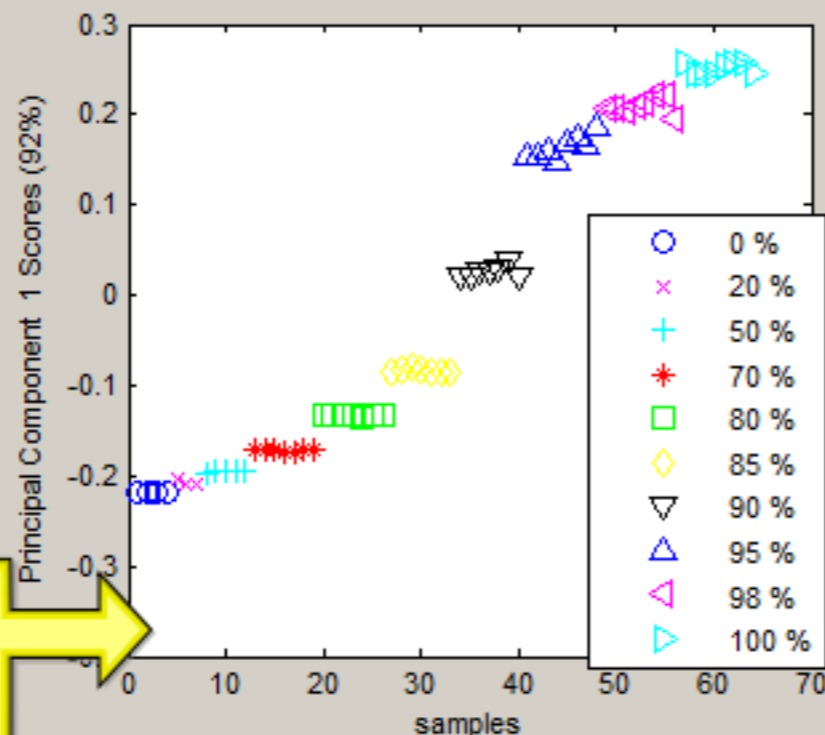
Name of Data Matrix:
 Name of Variable Matrix:
 Name of Filename Matrix:
 Name of Totalcounts Matrix:
 Name of Samplenames Matrix:

Load Selected Data

Image: **ndatassp**
 Variable: **exactmass**
 Scores: **scores**
 Loads: **loads**

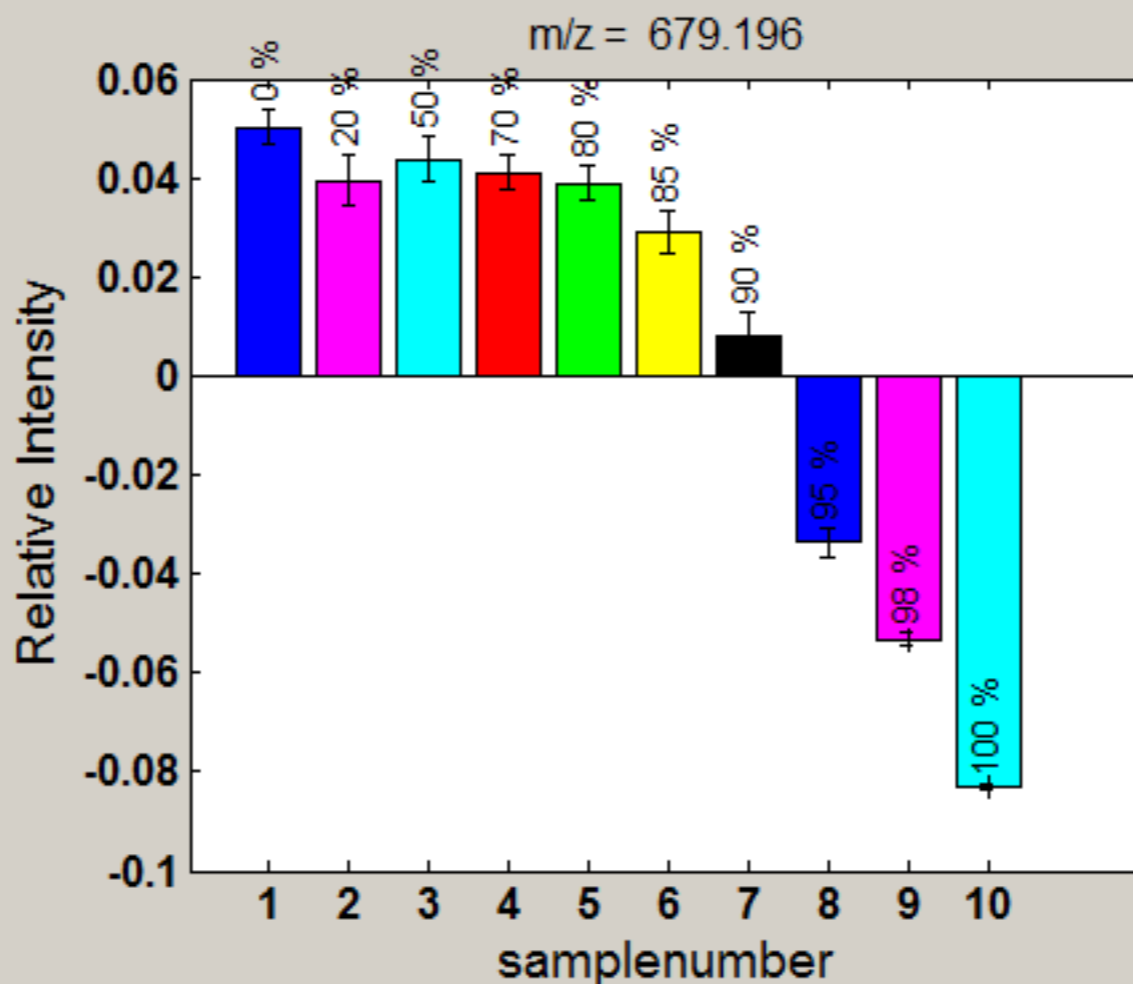
Data Preprocessing

PC #



Here I have gone back and plotted another peak for PC1. In this case I chose the m/z 679 peak which shows a high negative loading.

As expected the data for the m/z 679 peak shows an inverse trend as seen in the PC1 scores (since it has a negative loading).



Save Figure

Make Ext

Close Panel

655.3643--Au[M-H]2C
 679.196--Au2[M-H]C
 686.8168--unknown
 718.789--unknown
 767.498--Au[M-H]2C

Select Plot Type

Plot Peak Area Image

This plot will show the scaled for the selected peak after subtracting the PCs selected above.

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:

Load Selected Data

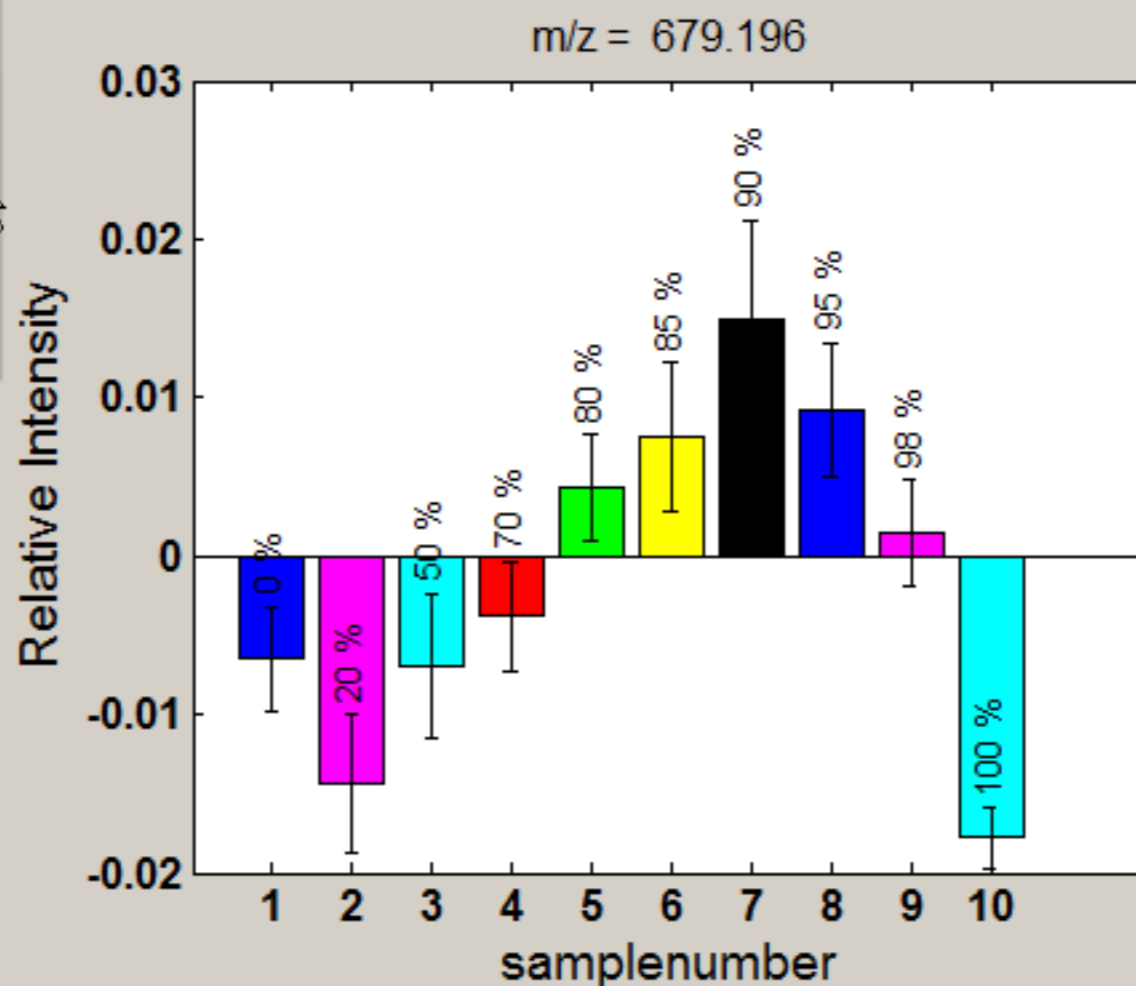
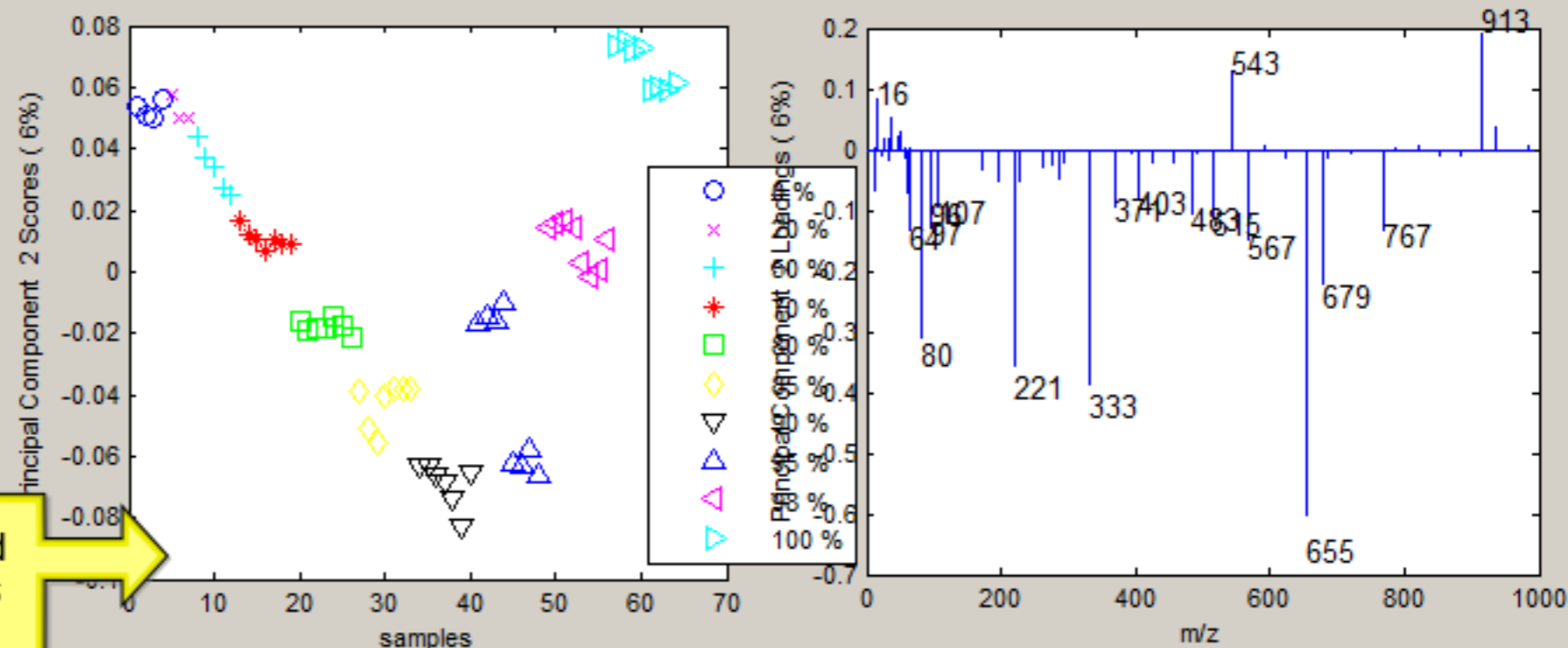
Image: **ndatassp**
 Variable: **exactmass**
 Scores: **scores**
 Loads: **loads**

Data Preprocessing

PC #

Here I plotted the m/z 679 pre-processed peak area data for PC2. On PC2 this peak also shows a negative loading.

The m/z 679 peak shows an inverse trend as seen in the PC2 scores (since it has a negative loading). The trend makes sense based off the PC2 scores.



Save Figure

Make Ext

Close Panel

- 655.3643--Au[M-H]2C
- 679.196--Au2[M-H]C
- 686.8168--unknown
- 718.789--unknown
- 767.498--Au[M-H]2C

Select Plot Type

Plot Peak Area Image

This plot will show the scaled for the selected peak after subtracting the PCs selected above.

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:

Load Selected Data

Image: **ndatassp**
 Variable: **exactmass**
 Scores: **scores**
 Loads: **loads**

Data Preprocessing

PC #

Plot Scores and Loads

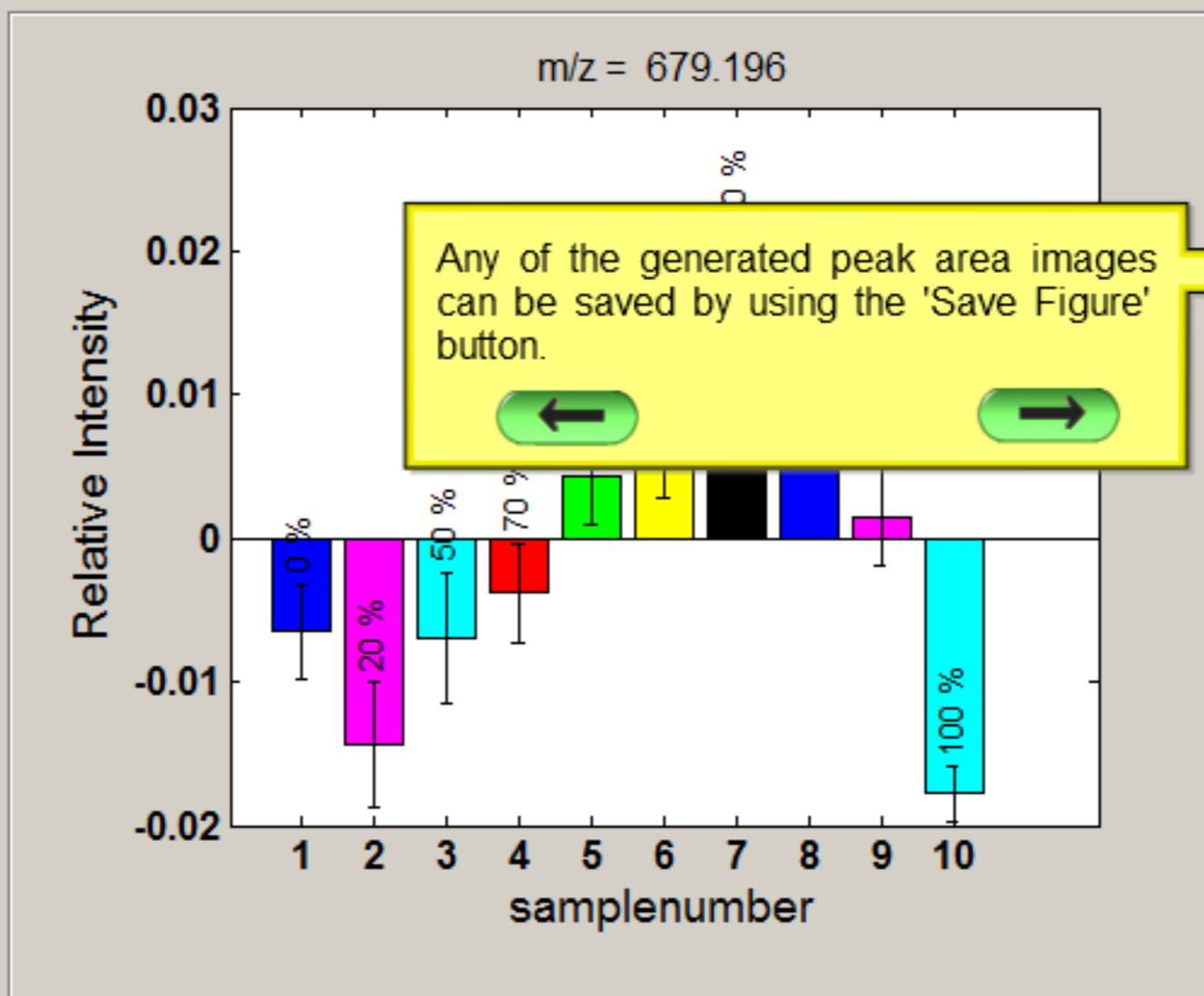
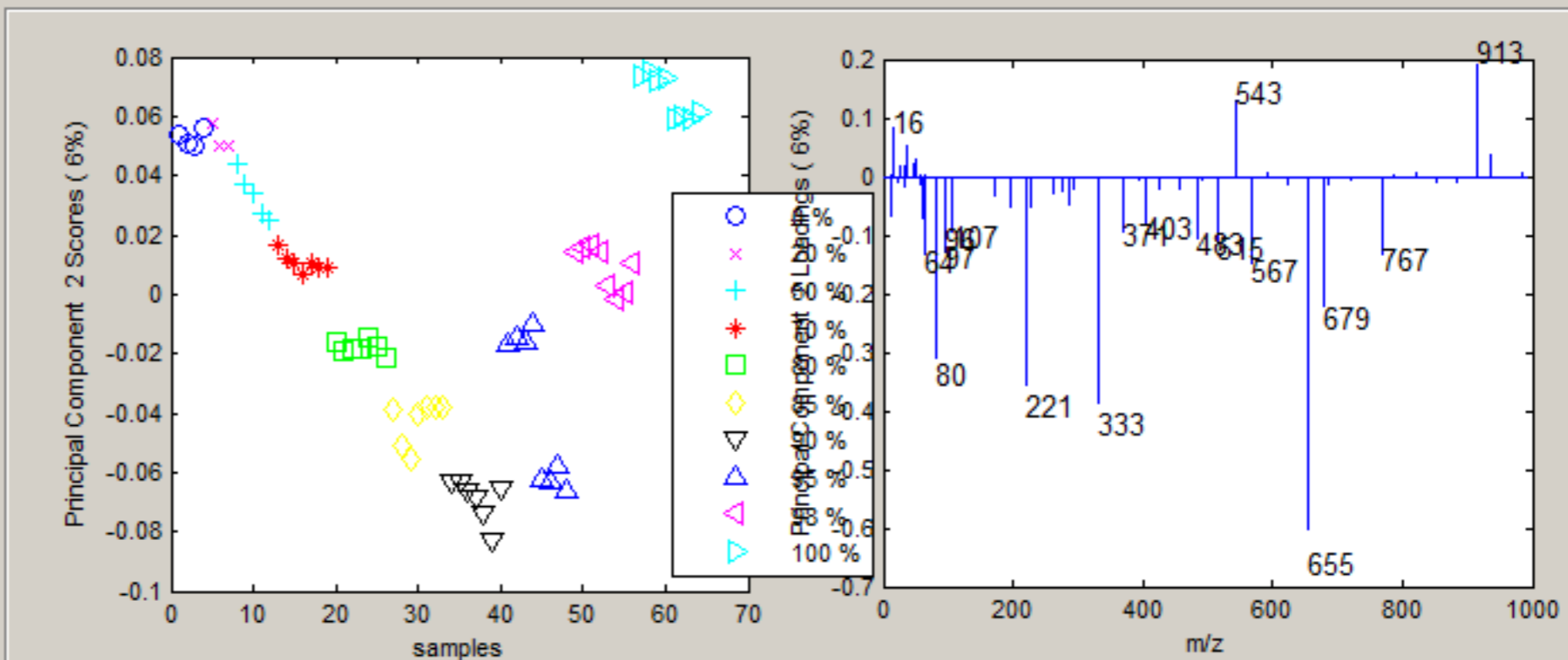
Peak List

- 489.8492--Au2S3
- 515.2086--Au[M-H]2C
- 543.2399--Au[M-H]2C
- 567.0683--Au2[M-H]C
- 590.8999--Au3
- 622.869--Au3S
- 654.8471--Au3S2O2I
- 655.3643--Au[M-H]2C
- 679.196--Au2[M-H]C
- 686.8168--unknown
- 718.789--unknown
- 767.498--Au[M-H]2C

Select Plot Type

Plot Peak Area Image

This plot will show the scaled for the selected peak after subtracting the PCs selected above.



Save Figure

Make Ext

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:

Load Selected Data

Image: **ndatassp**
 Variable: **exactmass**
 Scores: **scores**
 Loads: **loads**

Data Preprocessing

PC #

Plot Scores and Loads

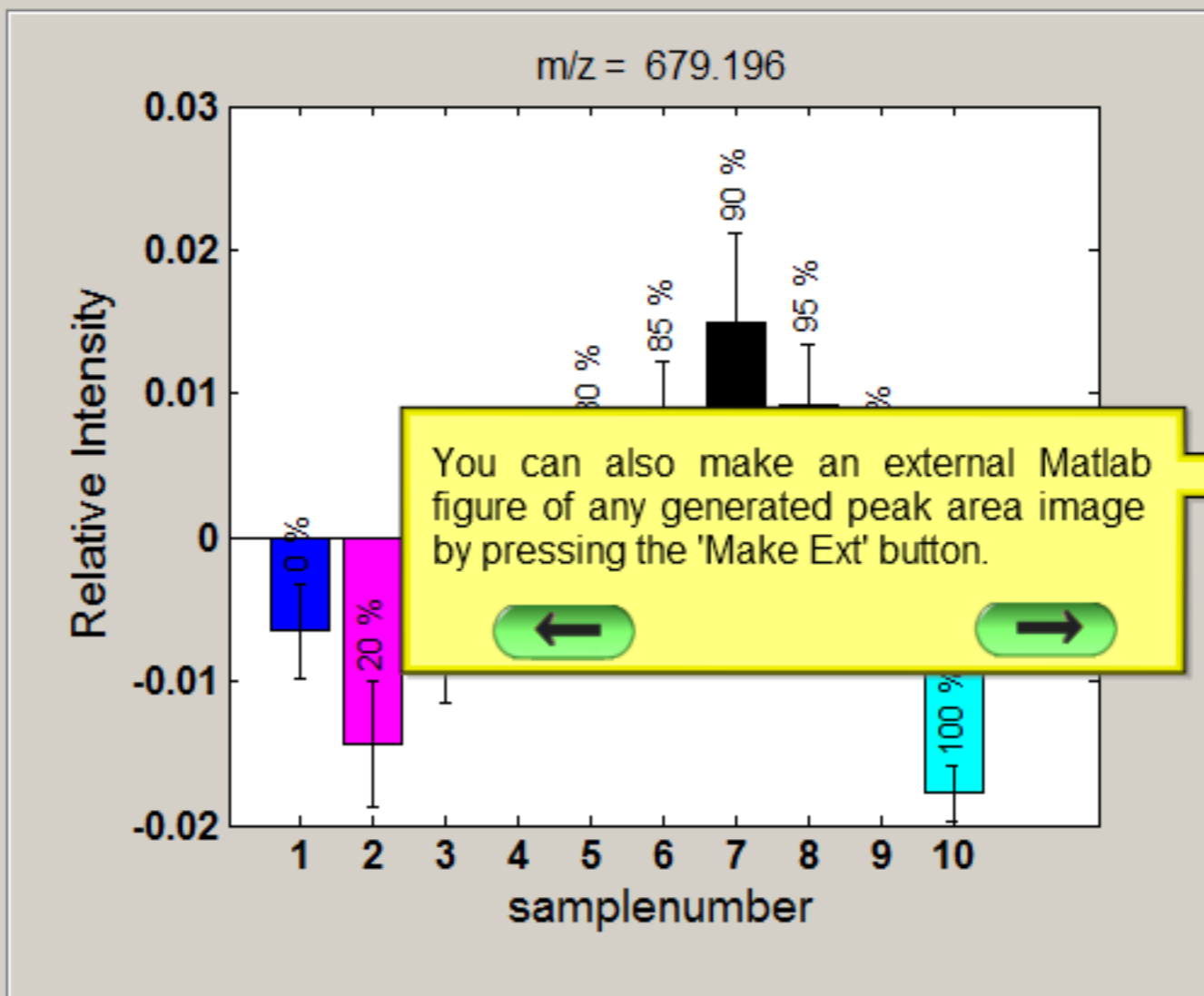
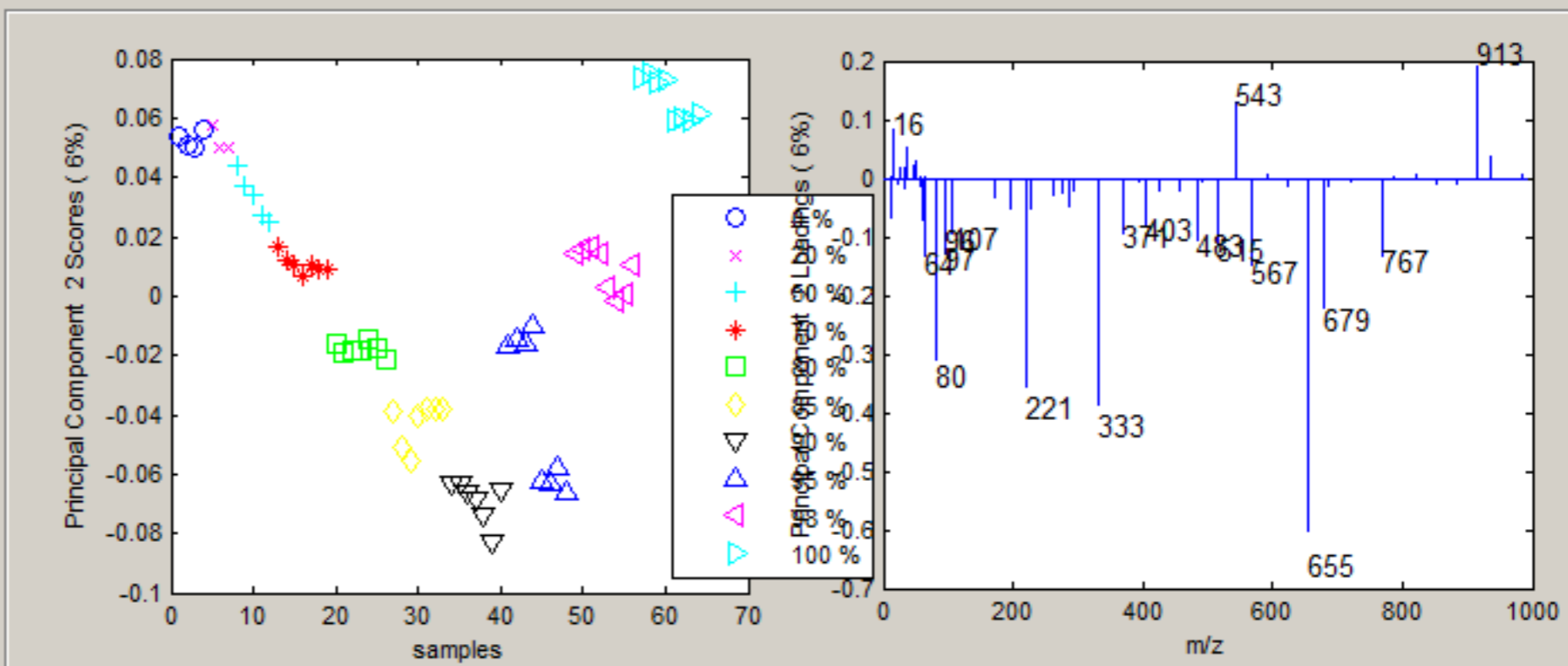
Peak List

- 489.8492--Au2S3
- 515.2086--Au[M-H]2C
- 543.2399--Au[M-H]2C
- 567.0683--Au2[M-H]C
- 590.8999--Au3
- 622.869--Au3S
- 654.8471--Au3S2O2I
- 655.3643--Au[M-H]2C
- 679.196--Au2[M-H]C
- 686.8168--unknown
- 718.789--unknown
- 767.498--Au[M-H]2C

Select Plot Type

Plot Peak Area Image

This plot will show the scaled for the selected peak after subtracting the PCs selected above.



Save Figure

Make Ext

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:

Load Selected Data

Image: **ndatassp**
Variable: **exactmass**
Scores: **scores**
Loads: **loads**

Data Preprocessing

PC #

Plot Scores and Loads

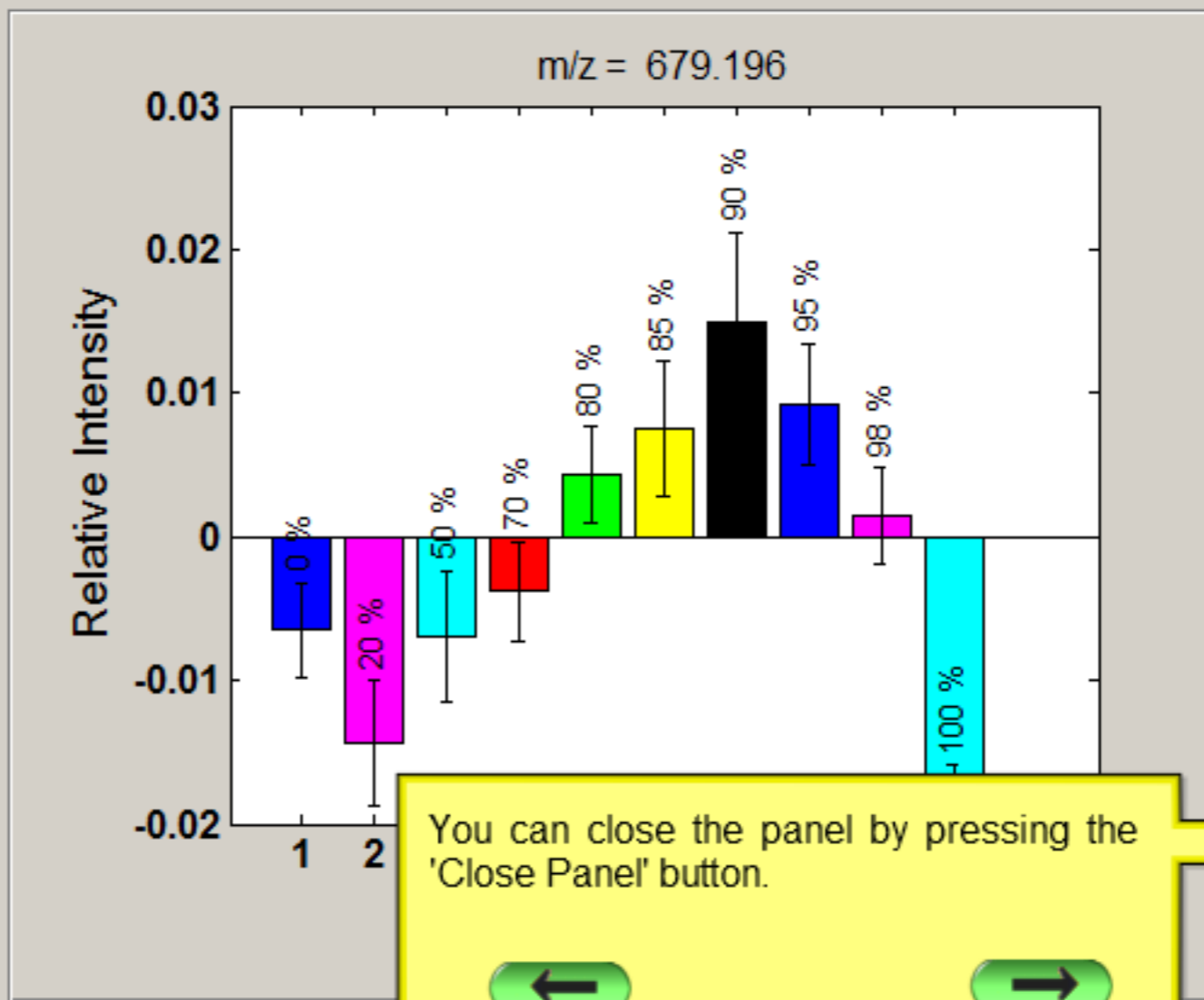
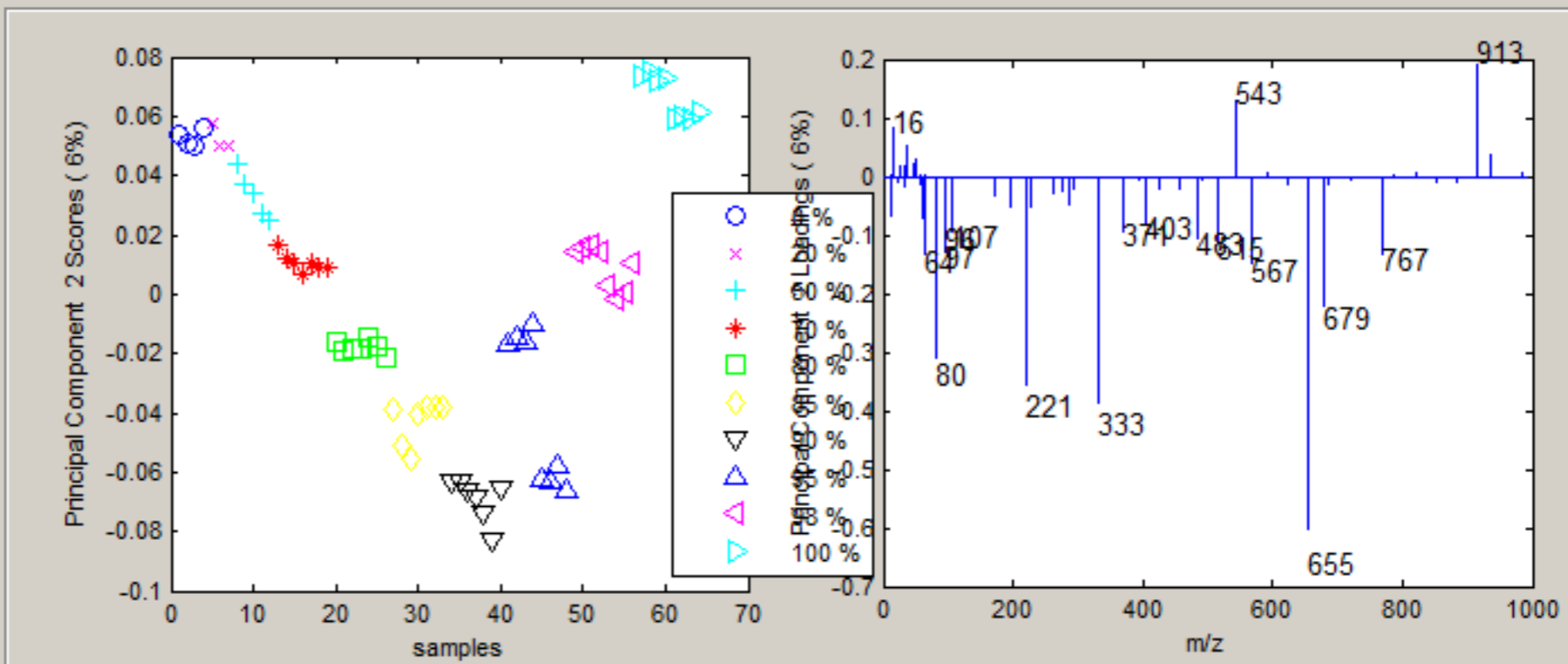
Peak List

- 489.8492--Au2S3
- 515.2086--Au[M-H]20
- 543.2399--Au[M-H]20
- 567.0683--Au2[M-H]C
- 590.8999--Au3
- 622.869--Au3S
- 654.8471--Au3S2O2I
- 655.3643--Au[M-H]20
- 679.196--Au2[M-H]C
- 686.8168--unknown
- 718.789--unknown
- 767.498--Au[M-H]20

Select Plot Type

Plot Peak Area Image

This plot will show the scaled for the selected peak after subtracting the PCs selected above.



Save Figure

Make Ext

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

That ends this tutorial. Press the button on the left to go back to the previous step. Press the button on the right to start the tutorial over.

