

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

Select Data

Select Variables

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

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

PCA_scores

Loadings

PCA_loads

Variance

PCA_va

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).

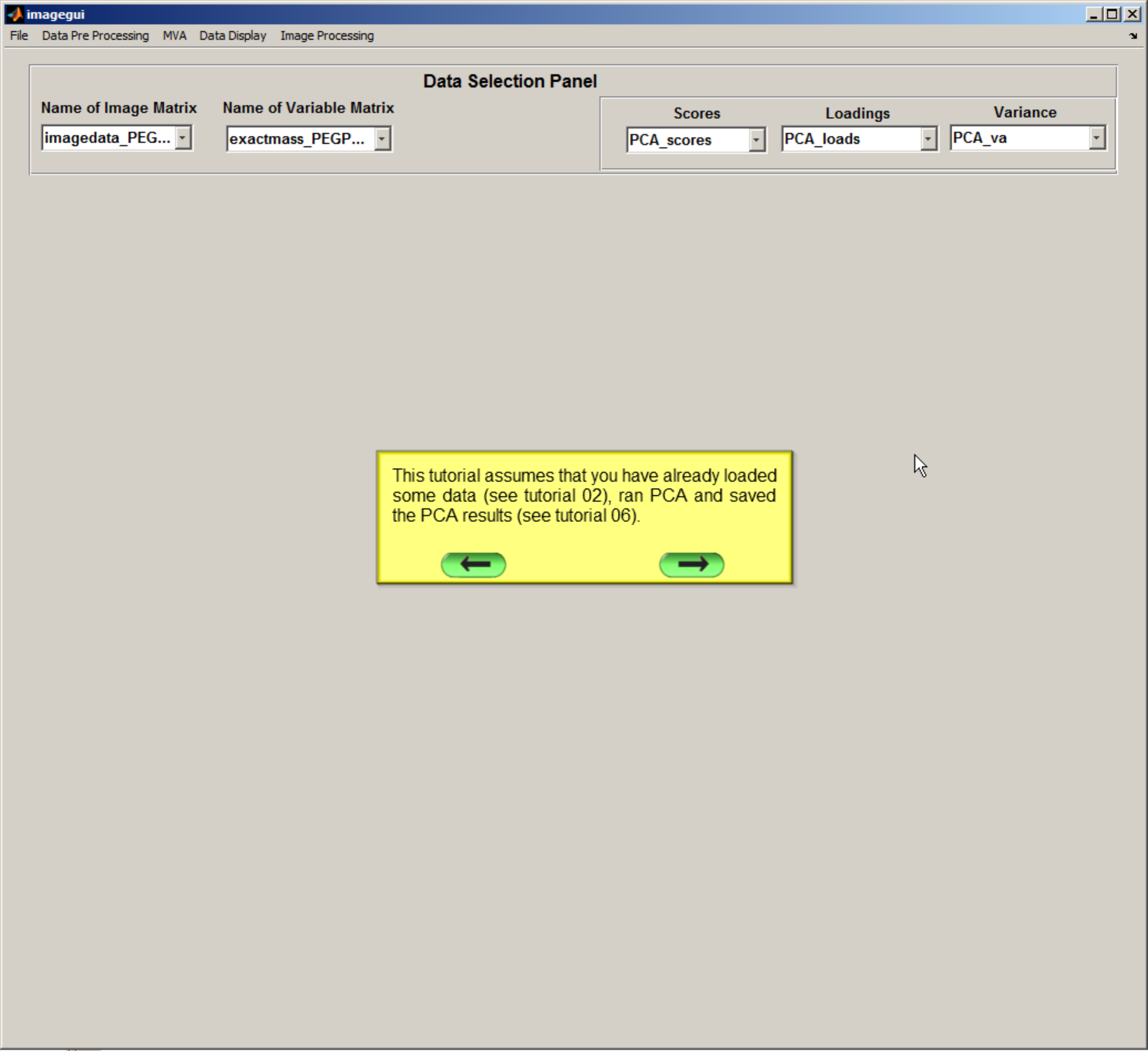
In this tutorial I will provide examples of how this works and why it can be useful.

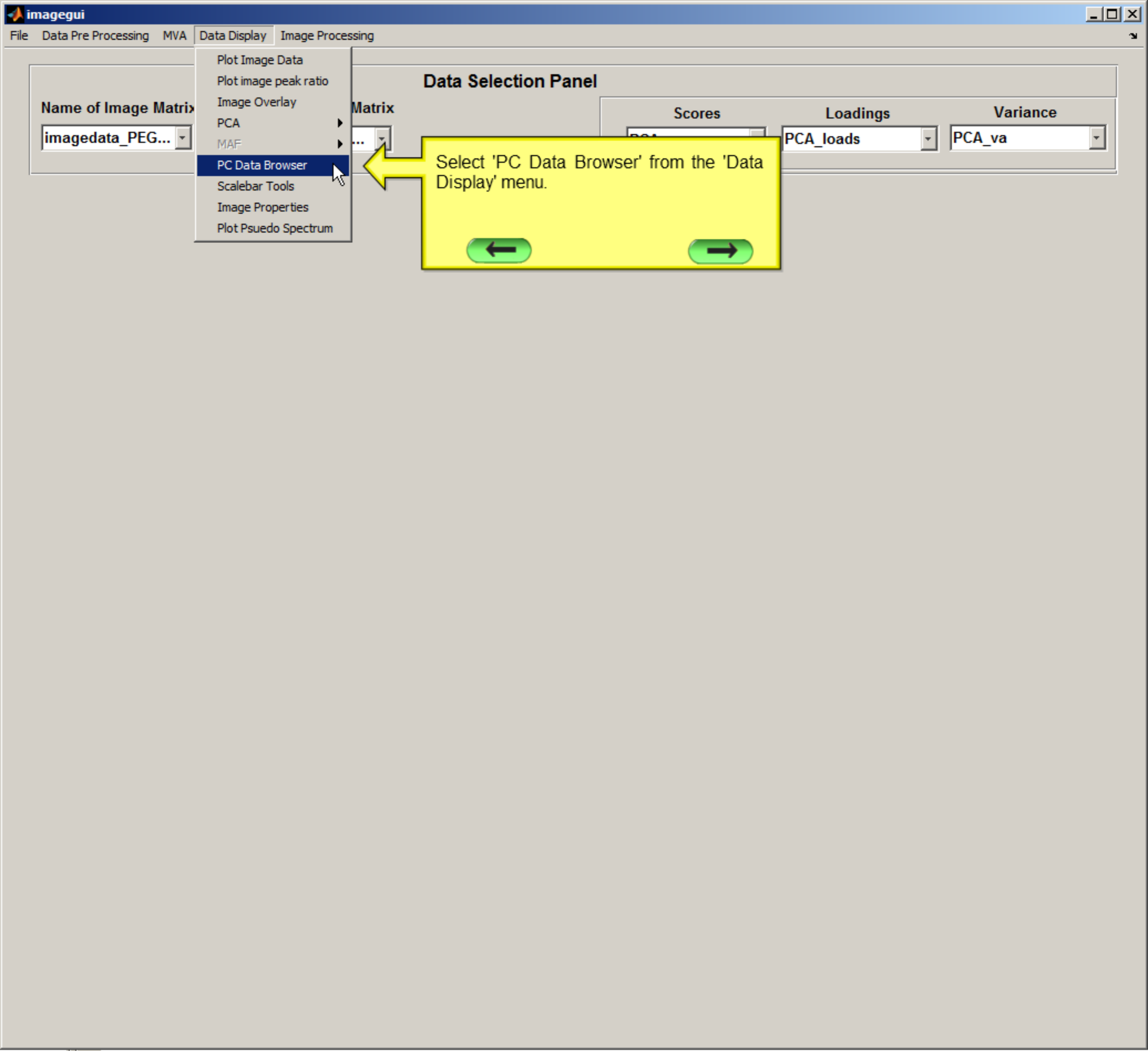
$$X = T_1 P_1^T + E$$

Residual becomes new X matrix

$$X - T_1 P_1^T$$

$$X = T_2 P_2^T + E$$





Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

Select the saved PCA data from each menu on the right.

Load Sele

Image:

Variables

Scores:

Loads:

None

None

None

Data Preprocessing

Choose an option below

PC #

Choose one:

PCA Plot Options: Traditional

Plot Scores and Loads

Peak List

Empty list box for Peak List

Plot Peak Area Image

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

Scores

Select Scores

Select Scores

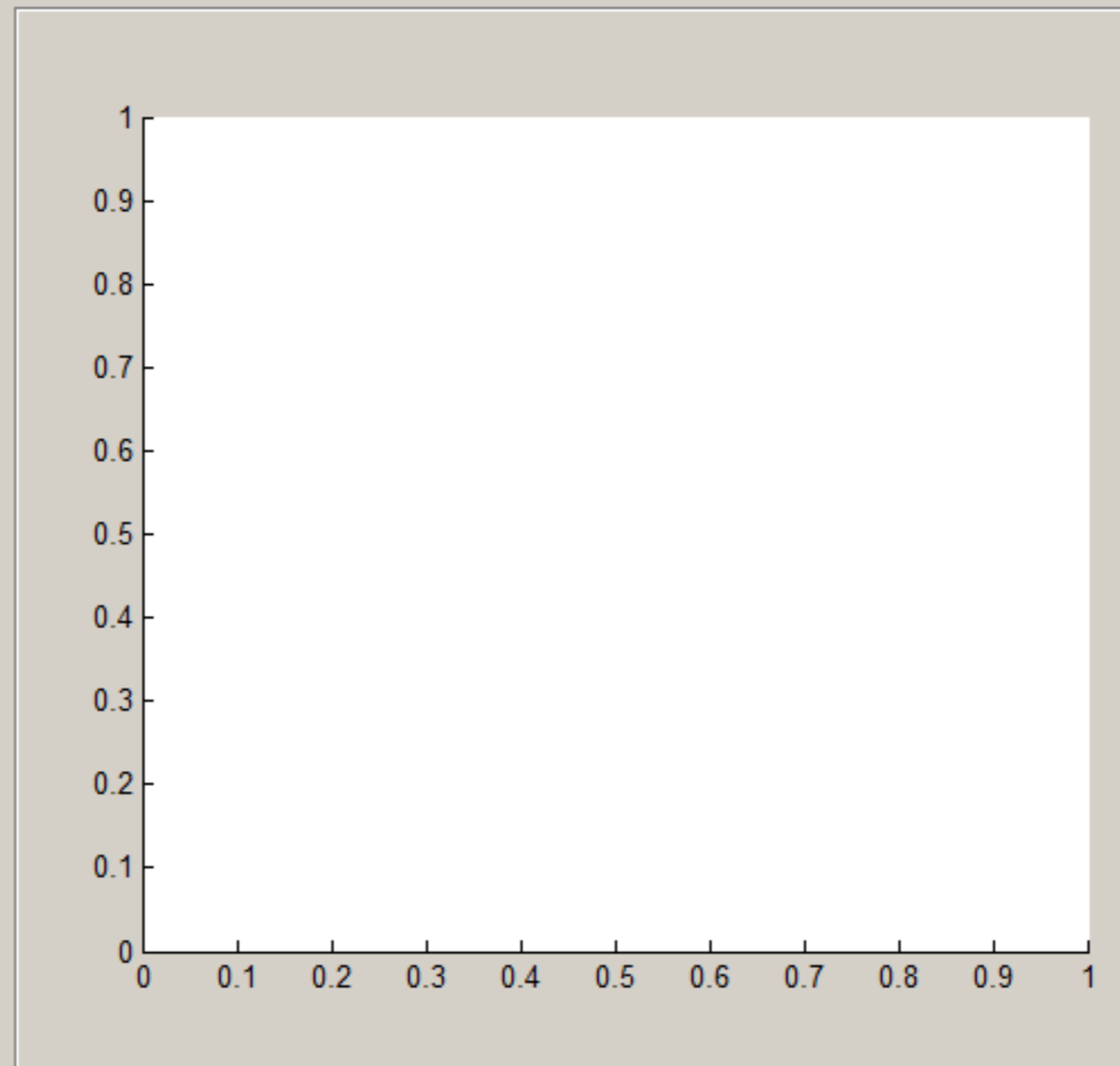
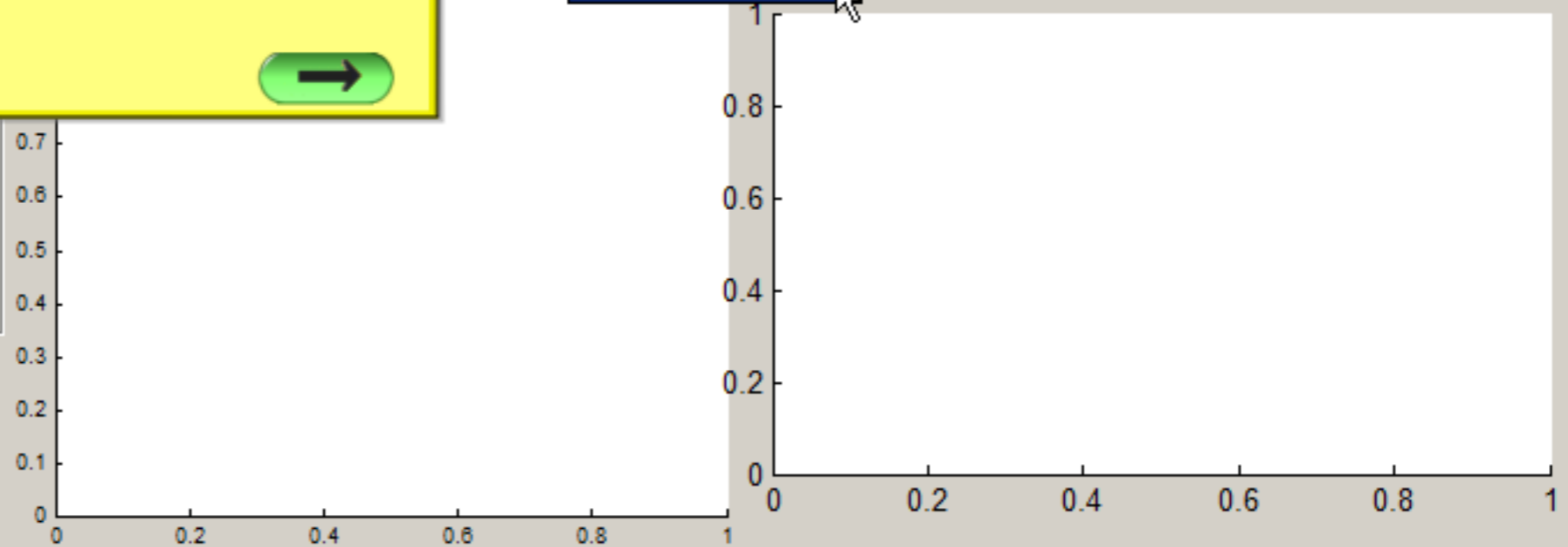
PCA_scores

Loadings

Select Loadings

Variance

Select Variance



Save Figure

Make Ext

Close Panel

Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

PCA_scores

Loadings

PCA_loads

Variance

PCA_va

Load Selected Data

Image:

None

Variables

None

Scores:

None

Loads:

None

Data Preprocessing

Choose an option below

PC #

Choose one:

PCA Plot Options: Traditional

Plot Scores and Loads

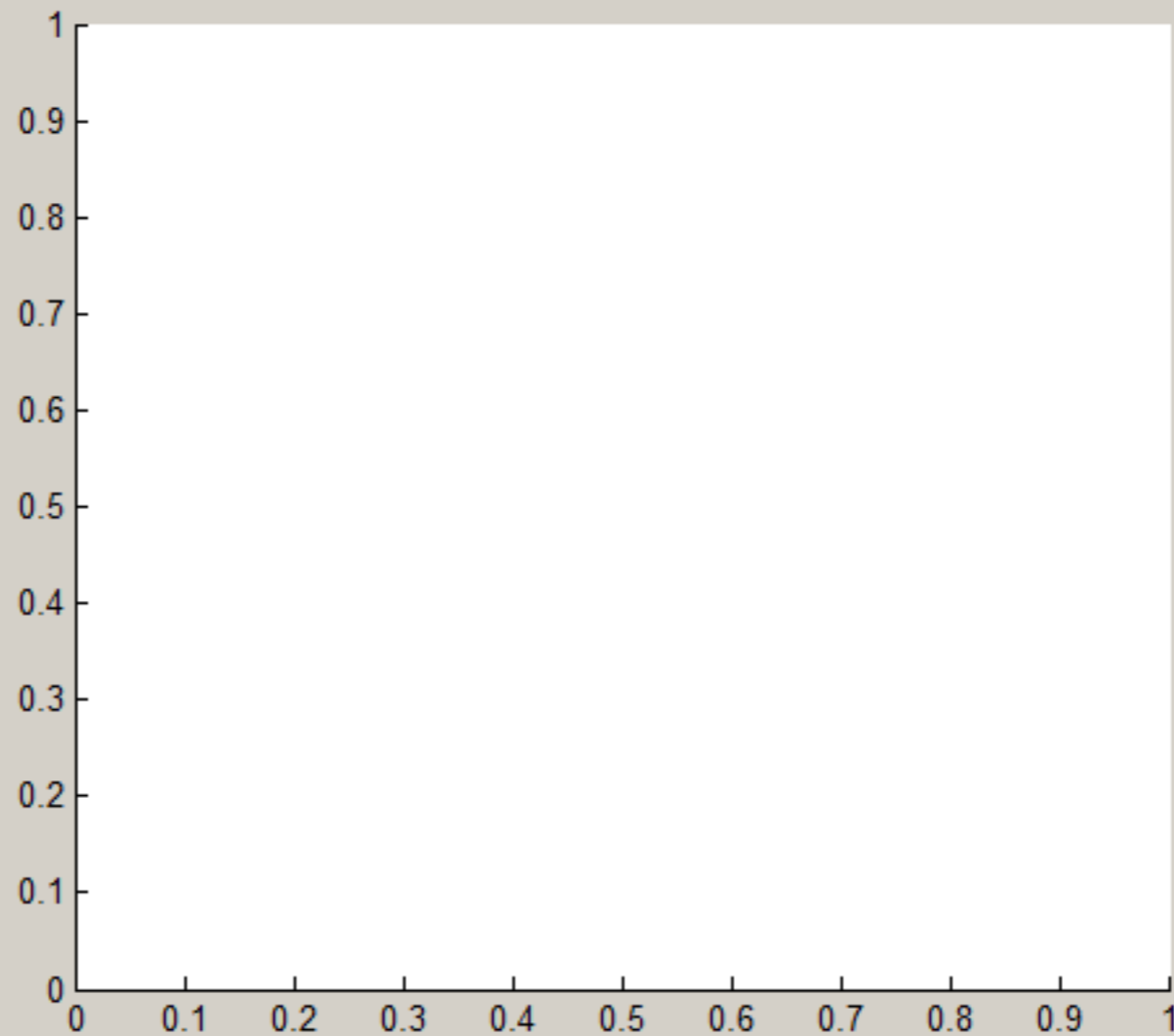
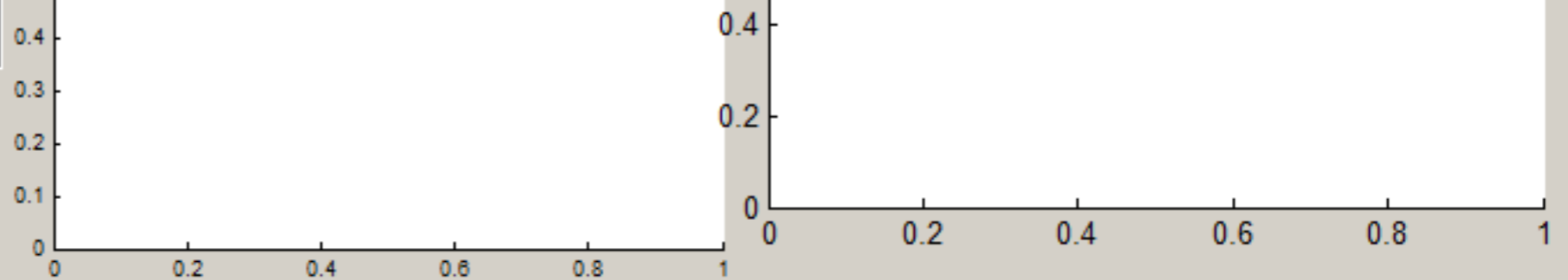
Peak List

Empty list box for Peak List

Plot Peak Area Image

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

Once all of the data is selected for both the
original data and the PCA results, press
the 'Load Selected Data' button.



Save Figure

Make Ext

Close Panel

Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

PCA_scores

Loadings

PCA_loads

Variance

PCA_va

Load Selected Data

Image: imagedata_PEGPS_07

Variables: exactmass_PEGPS_07

Scores: PCA_scores

Loads: PCA_loads

Data Preprocessing

Choose an option below

Choose an option below

None

Autoscale

Mean Center

Squareroot

Squareroot & mean center

Poisson Scaling

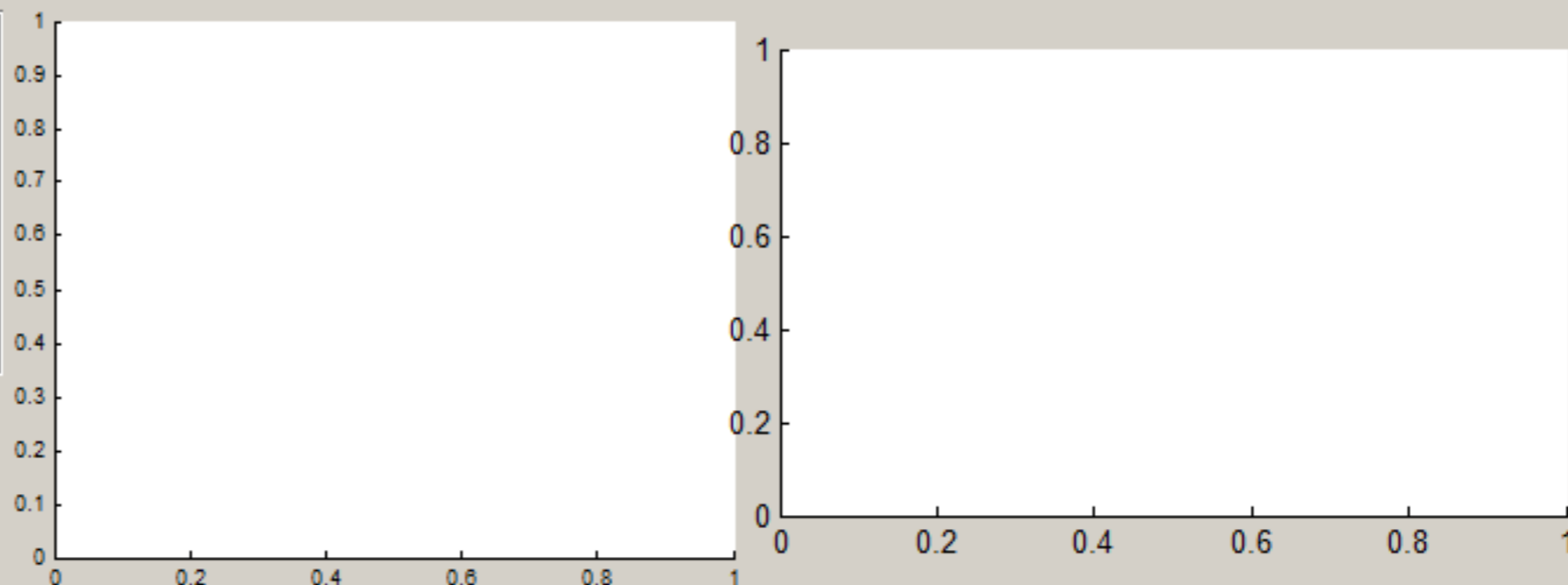
PoissonScaling & Mean Center

Mass scale

Mass scale & Mean Center

Mass^2 scale

Mass^2 scale & Mean Center

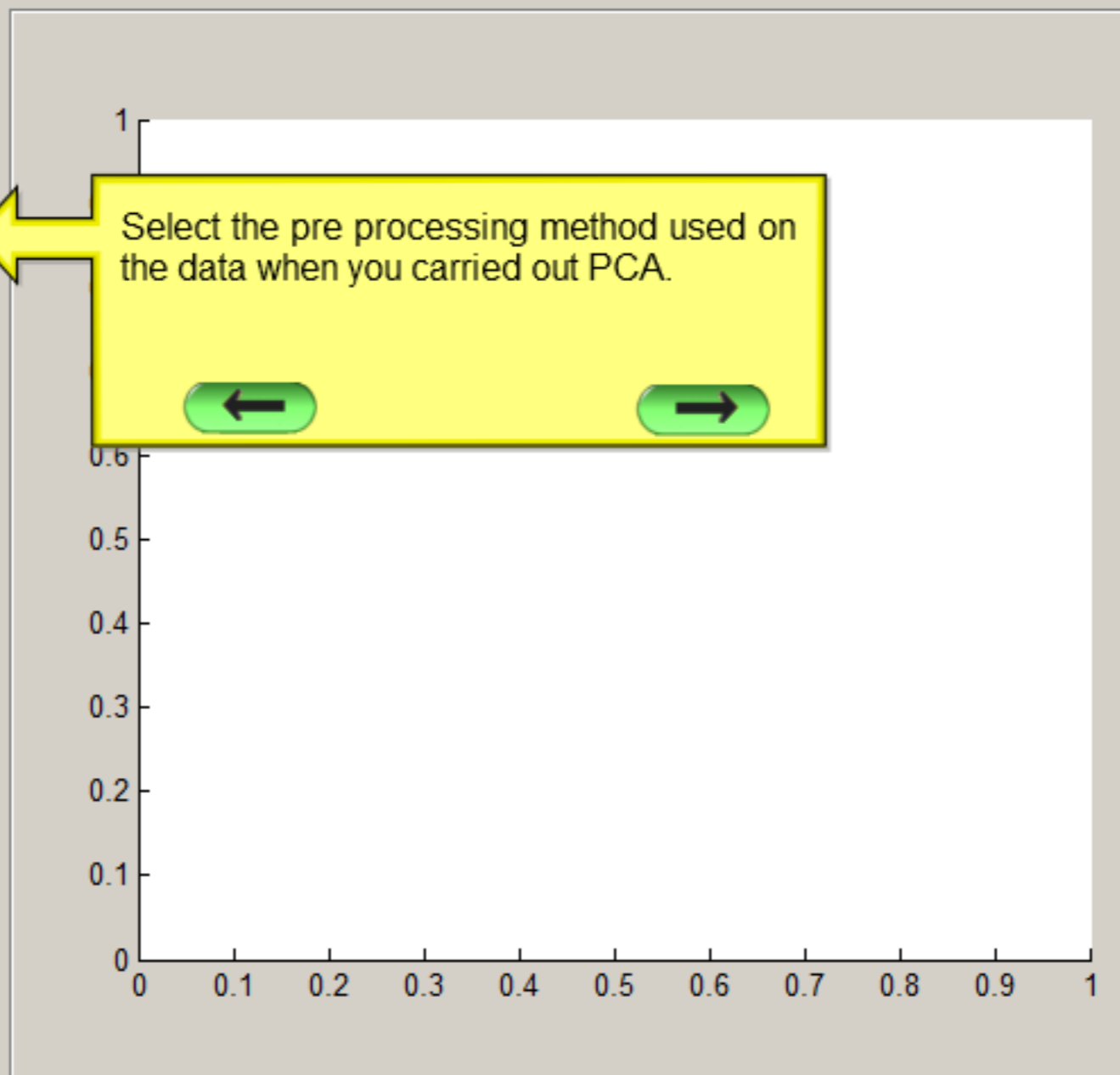


PCA P

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

Save Figure

Make Ext



Plot Peak Area Image

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

Close Panel

Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

PCA_scores

Loadings

PCA_loads

Variance

PCA_va

Load Selected Data

Image: imagedata_PEGPS_07

Variables: exactmass_PEGPS_07

Scores: PCA_scores

Loads: PCA_loads

Data Preprocessing

PoissonScaling & Mean C...

PC #

1

Choose one:

1

2

3

4

PCA Plot C

PC

Peak List

18.9985

25.0083

27.9764

29.0035

30.9976

31.0197

34.9697

34.9923

36.0001

37.0082

37.9961

38.0159

39.0052

39.0251

39.9952

41.0043

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

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

PCA_scores

Loadings

PCA_loads

Variance

PCA_va

Load Selected Data

Image: imagedata_PEGPS_07

Variables: exactmass_PEGPS_07

Scores: PCA_scores

Loads: PCA_loads

Data Preprocessing

PoissonScaling & Mean C...

PC #

1

PCA Plot Options: Traditional

Plot Score

Traditional

Pos Scores Only

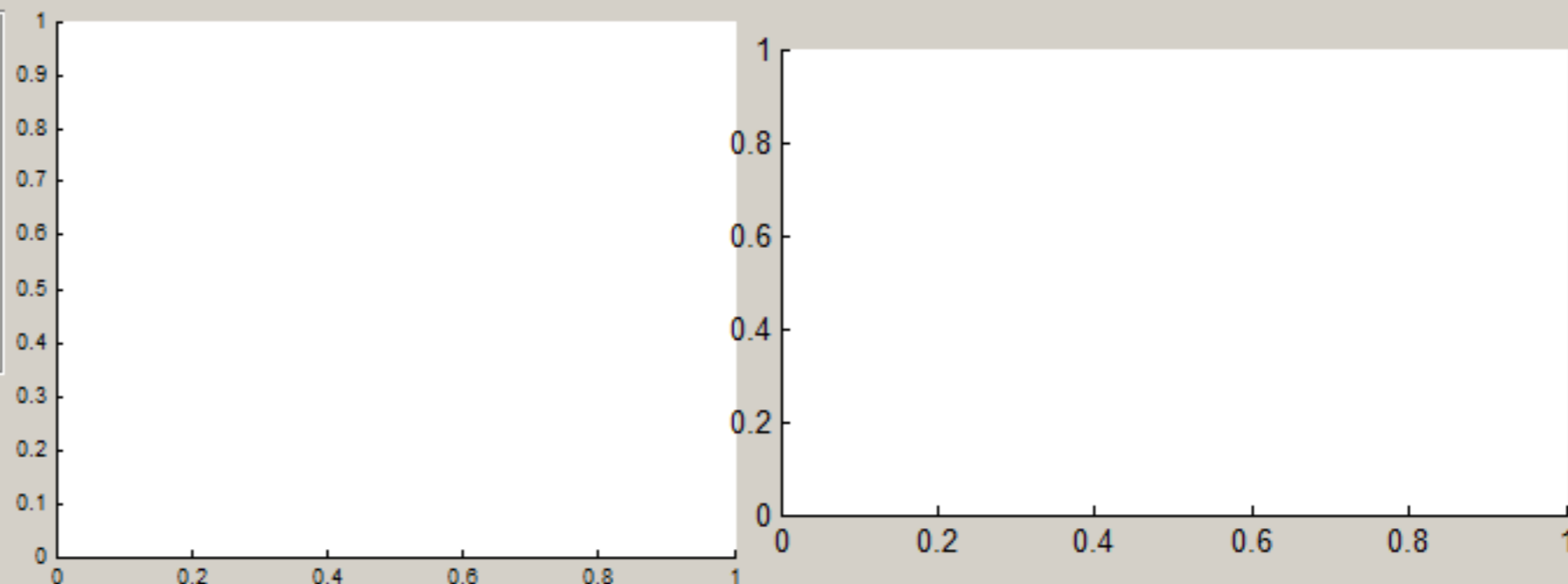
Neg Scores Only

Peak List

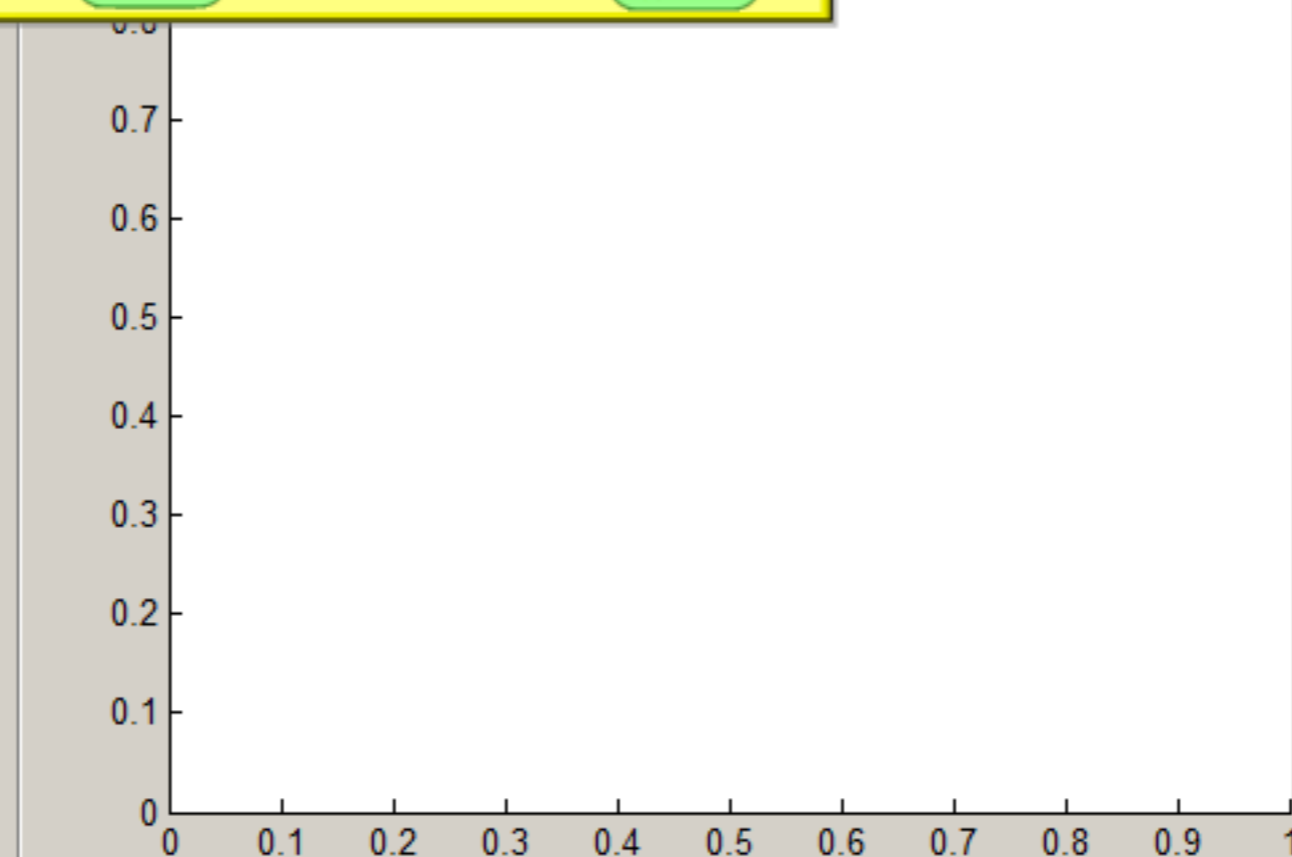
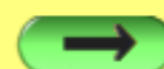
18.9985
25.0083
27.9764
29.0035
30.9976
31.0197
34.9697
34.9923
36.0001
37.0082
37.9961
38.0159
39.0052
39.0251
39.9952
41.0043

Plot Peak Area Image

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



You can choose which way you want to display the PCA results. We will choose to use a traditional view showing all scores and loadings.



Save Figure

Make Ext

Close Panel

Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

PCA_scores

Loadings

PCA_loads

Variance

PCA_va

Load Selected Data

Image: imagedata_PEGPS_07

Variables: exactmass_PEGPS_07

Scores: PCA_scores

Loads: PCA_loads

Data Preprocessing

PoissonScaling & Mean C...

PC #

1

PCA Plot Options: Traditional

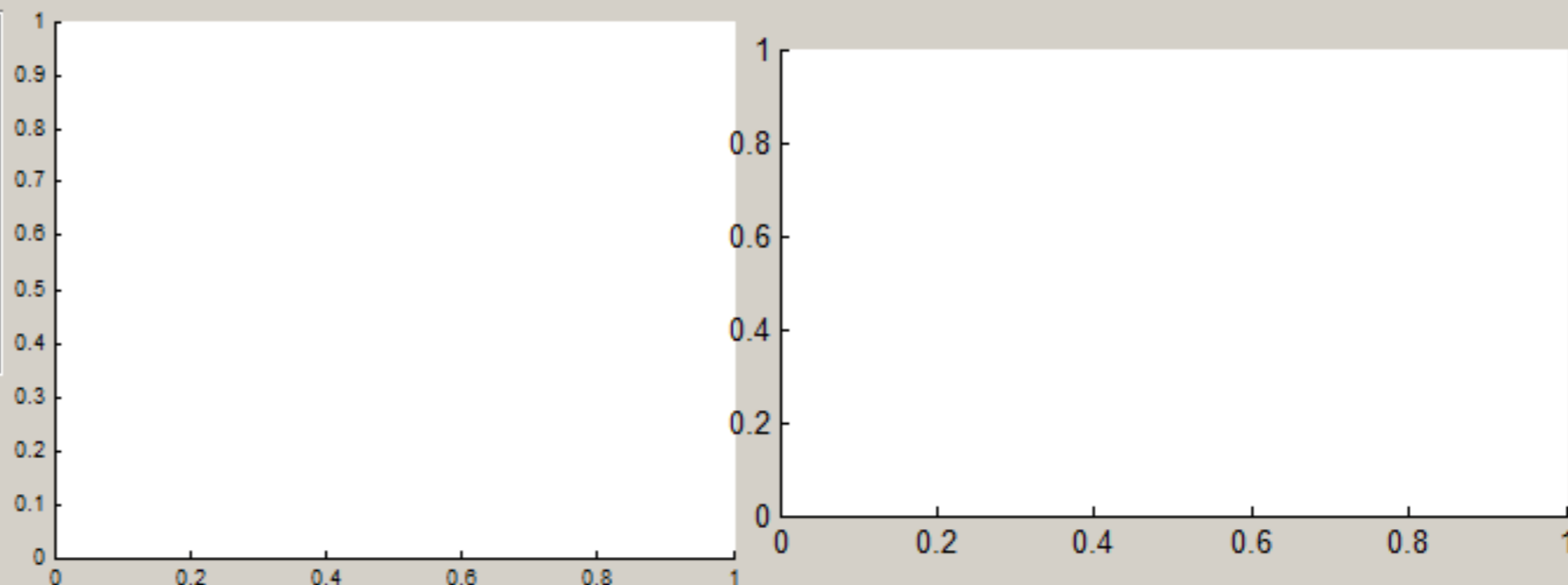
Plot Scores and Loads

Peak List

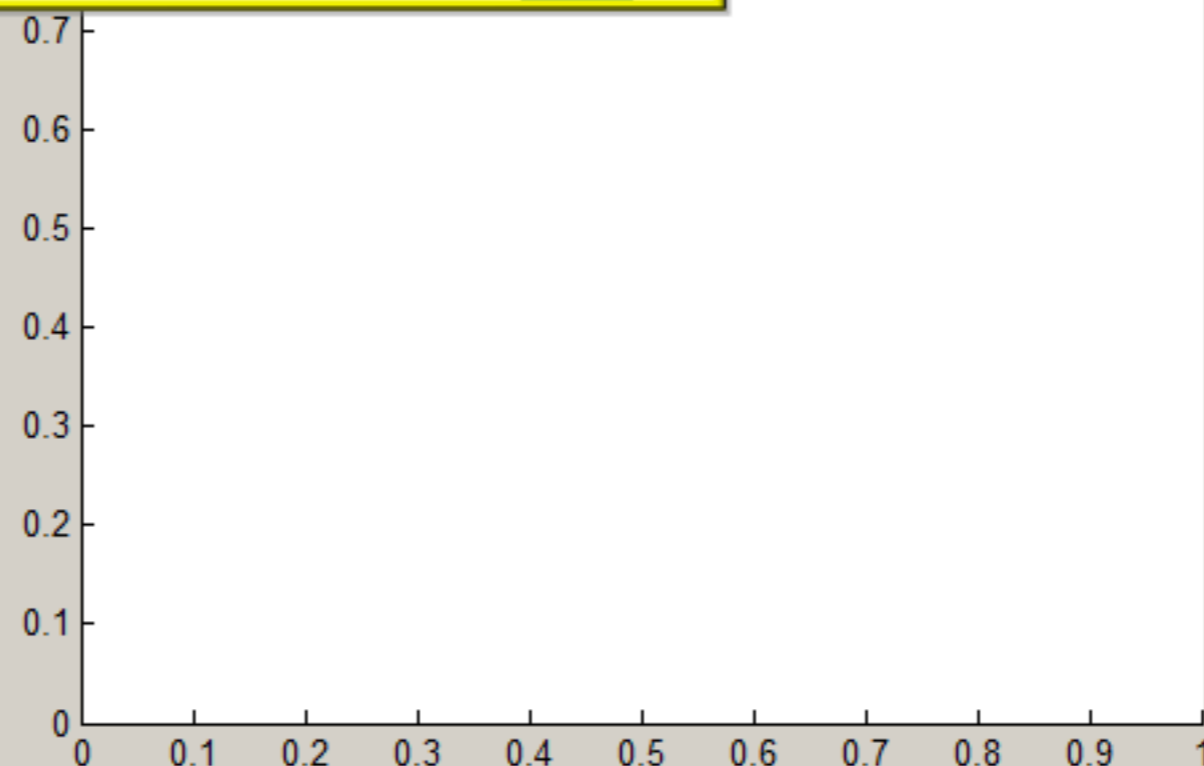
18.9985
25.0083
27.9764
29.0035
30.9976
31.0197
34.9697
34.9923
36.0001
37.0082
37.9961
38.0159
39.0052
39.0251
39.9952
41.0043

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

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

PCA_scores

Loadings

PCA_loads

Variance

PCA_va

Load Selected Data

Image: imagedata_PEGPS_07

Variables: exactmass_PEGPS_07

Scores: PCA_scores

Loads: PCA_loads

Data Preprocessing

PoissonScaling & Mean C...

PC #

1

PCA Plot Options: Traditional

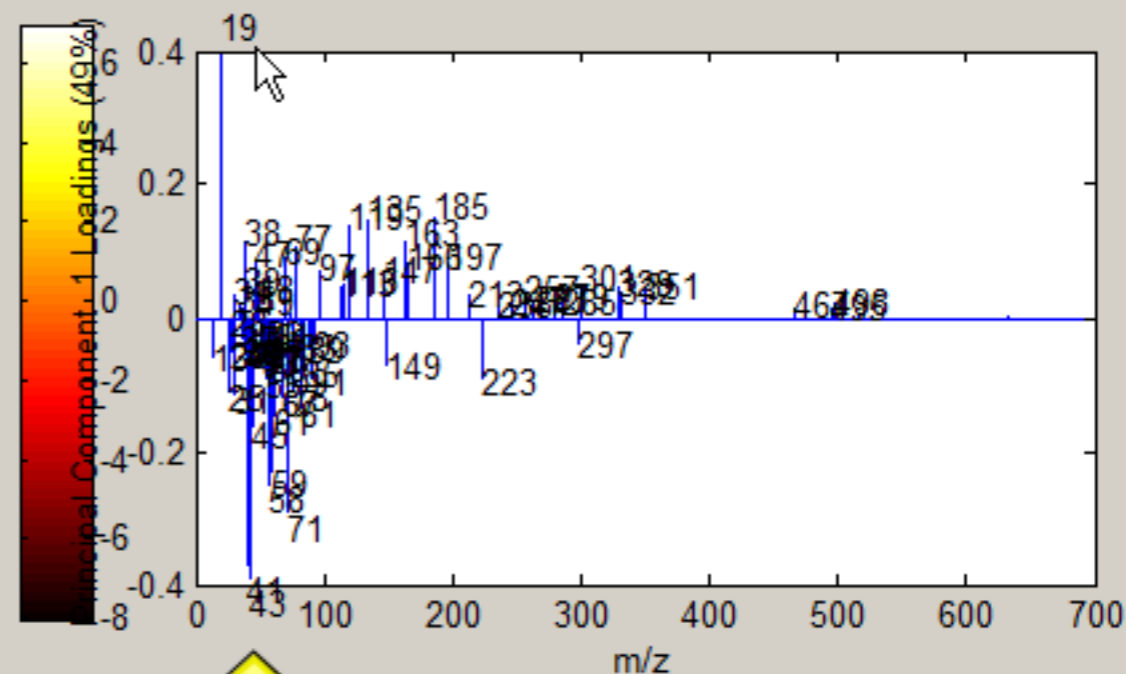
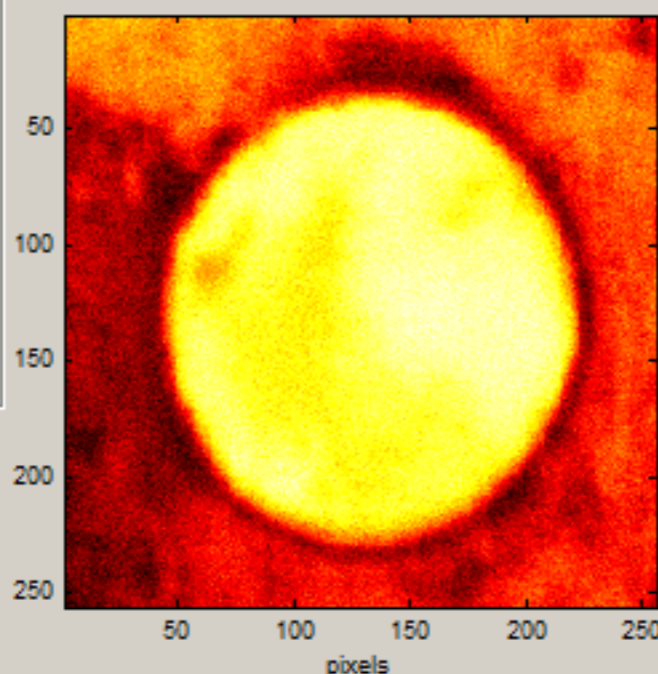
Plot Scores and Loads

Peak List

18.9985
25.0083
27.9764
29.0035
30.9976
31.0197
34.9697
34.9923
36.0001
37.0082
37.9961
38.0159
39.0052
39.0251
39.9952
41.0043

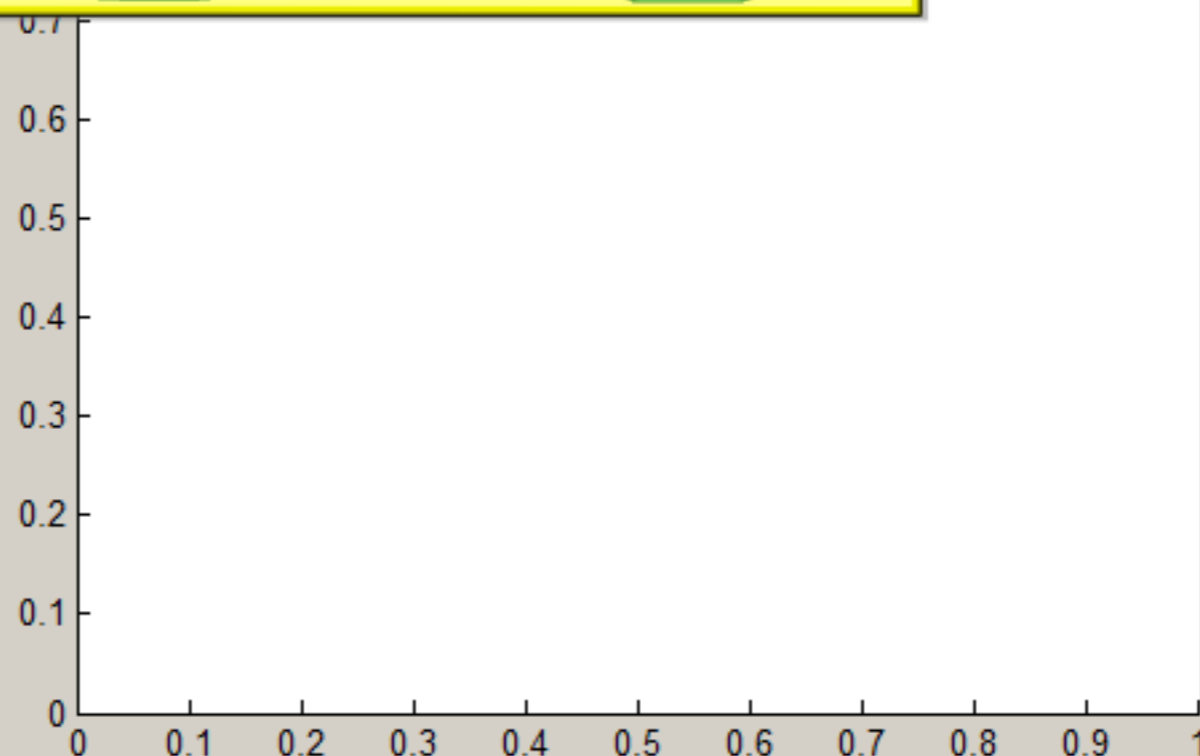
Plot Peak Area Image

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 19 has a high positive loading on PC1.



Save Figure

Make Ext

Close Panel

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

imagedata_PEG...

exactmass_PEGP...

Scores

Loadings

Variance

PCA_scores

PCA_loads

PCA_va

Load Selected Data

Image: imagedata_PEGPS_07

Variables: exactmass_PEGPS_07

Scores: PCA_scores

Loads: PCA_loads

Data Preprocessing

PoissonScaling & Mean C...

PC #

1

PCA Plot Options: Traditional

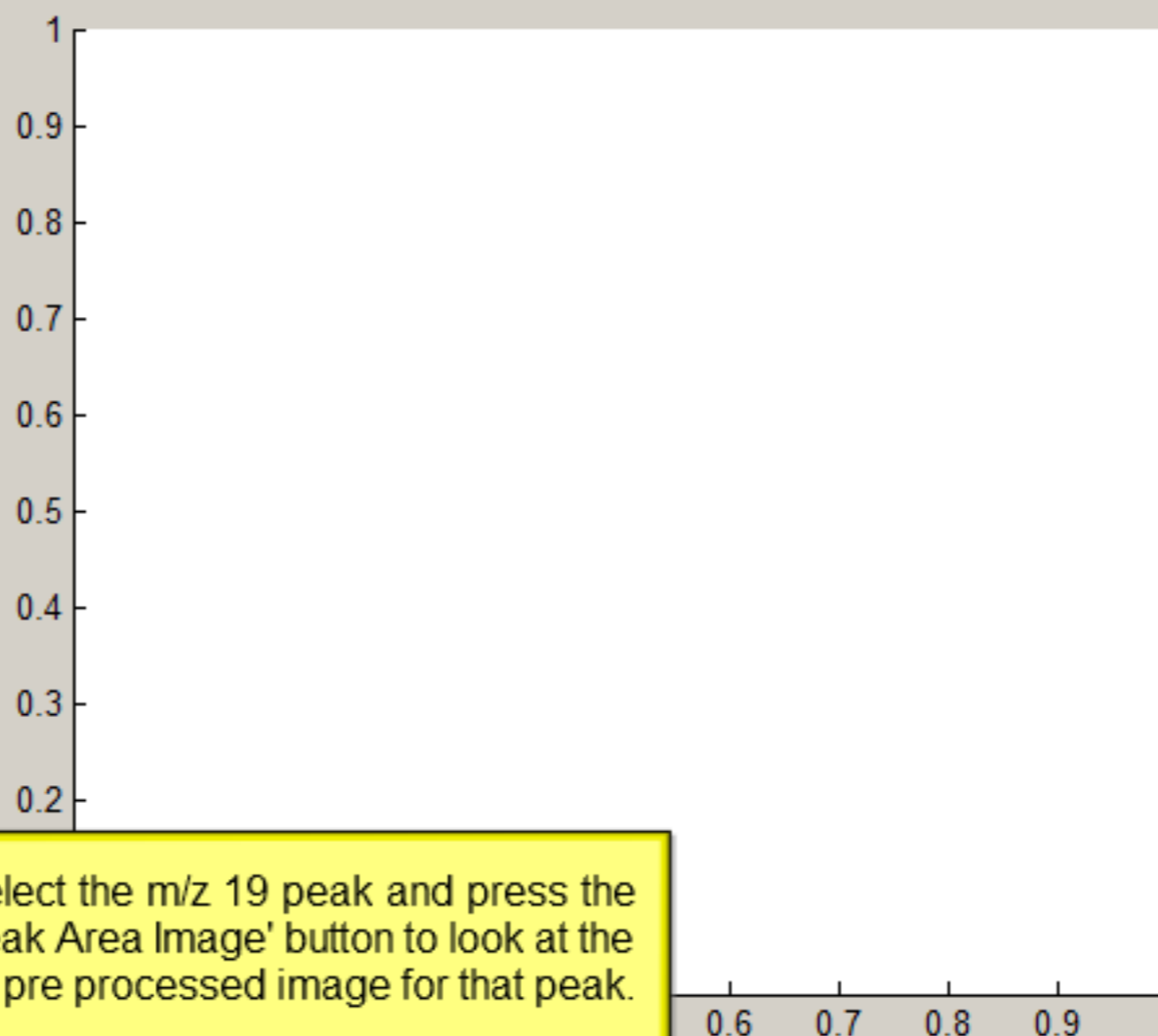
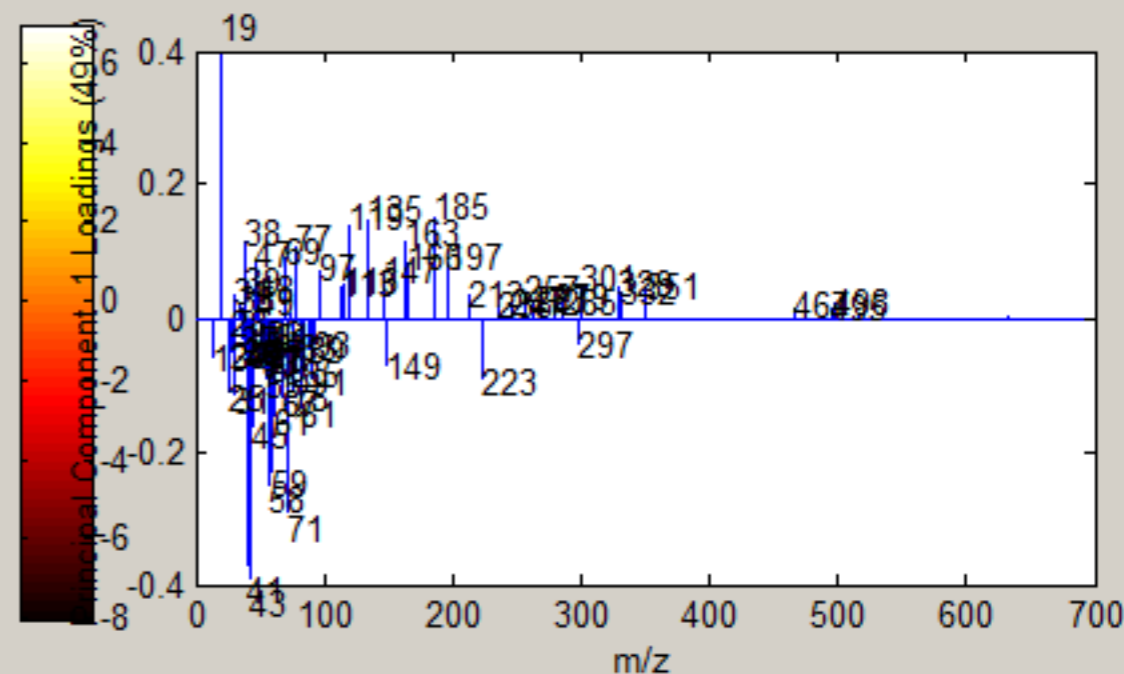
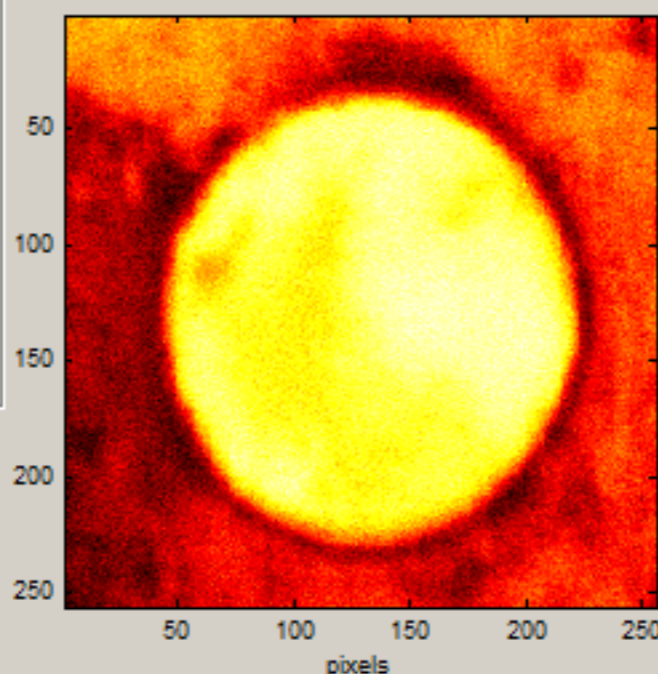
Plot Scores and Loads

Peak List

18.9985
25.0083
27.9764
29.0035
30.9976
31.0197
34.9697
34.9923
36.0001
37.0082
37.9961
38.0159
39.0052
39.0251
39.9952
41.0043

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 19 peak and press the
'Plot Peak Area Image' button to look at the
original pre processed image for that peak.



Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

imagedata_PEG...

exactmass_PEGP...

Scores

Loadings

Variance

PCA_scores

PCA_loads

PCA_va

Load Selected Data

Image: imagedata_PEGPS_07

Variables: exactmass_PEGPS_07

Scores: PCA_scores

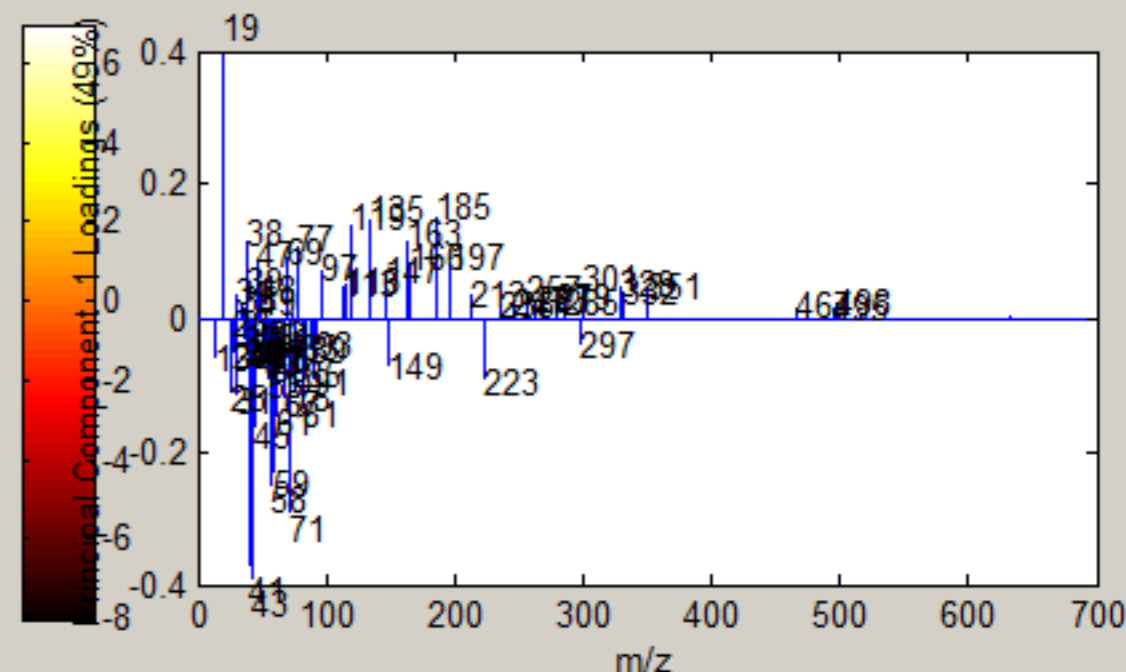
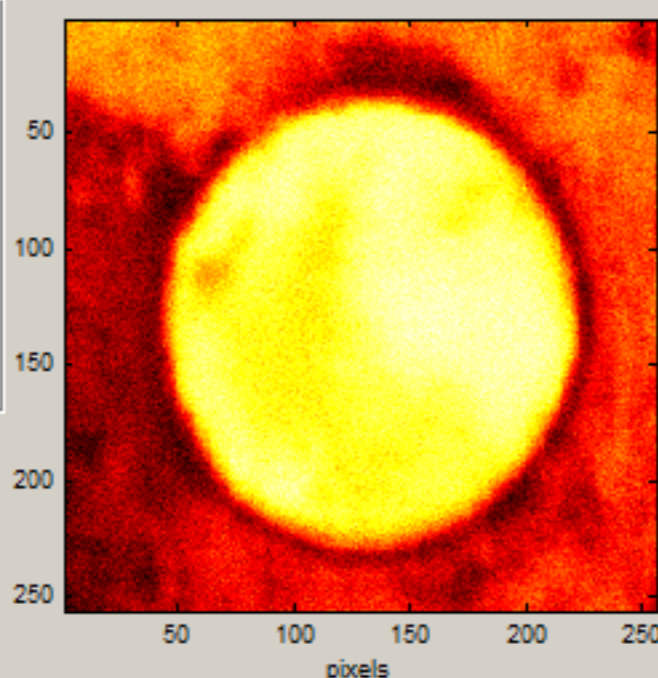
Loads: PCA_loads

Data Preprocessing

PoissonScaling & Mean C...

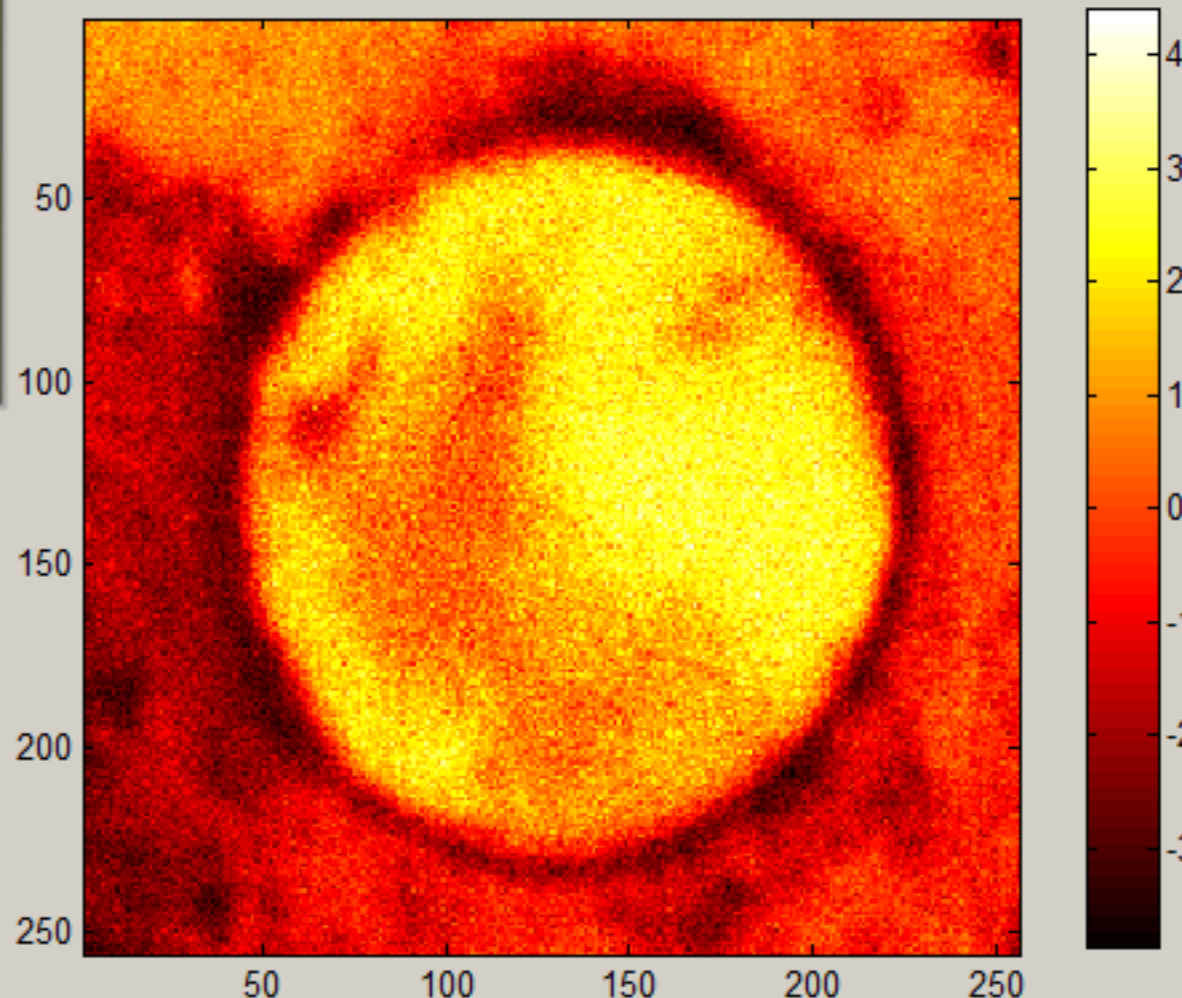
PC #

1



Here we see the pre processed image data for the m/z 19 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.

18.9985



Save Figure

Make Ext

Close Panel

Plot Peak Area Image

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

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

imagedata_PEG...

exactmass_PEGP...

Scores

Loadings

Variance

PCA_scores

PCA_loads

PCA_va

Load Selected Data

Image: imagedata_PEGPS_07

Variables: exactmass_PEGPS_07

Scores: PCA_scores

Loads: PCA_loads

Data Preprocessing

PoissonScaling & Mean C...

PC #

1

Choose one:

1

2

3

4

Peak List

18.9985

25.0083

27.9764

29.0035

30.9976

31.0197

34.9697

34.9923

36.0001

37.0082

37.9961

38.0159

39.0052

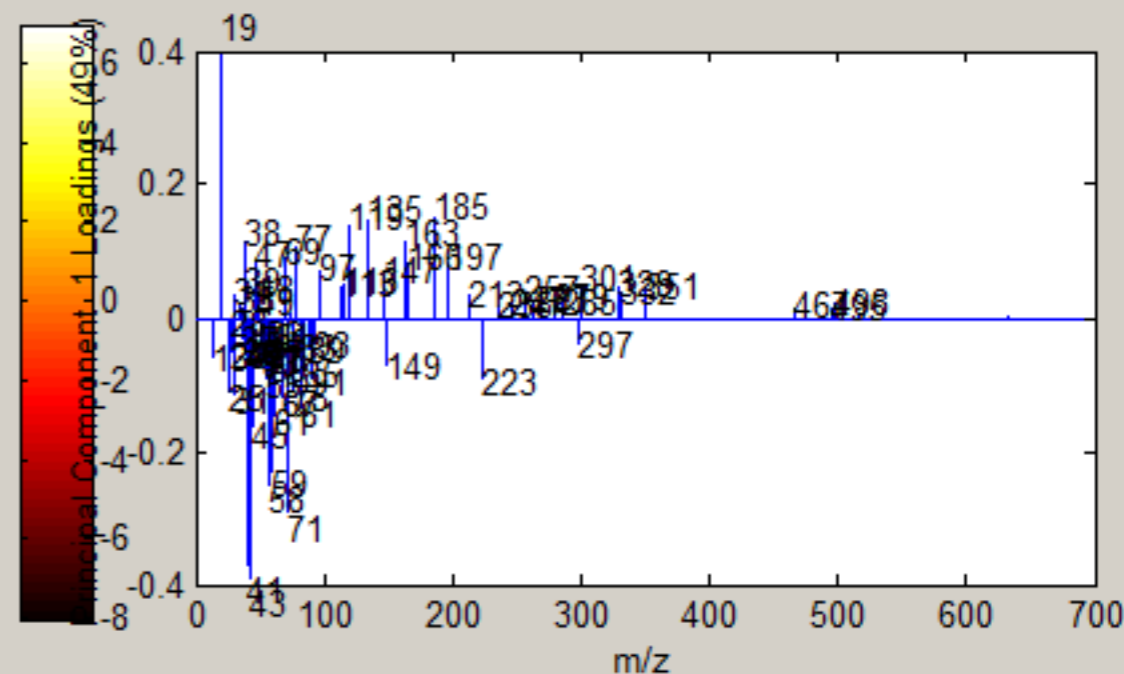
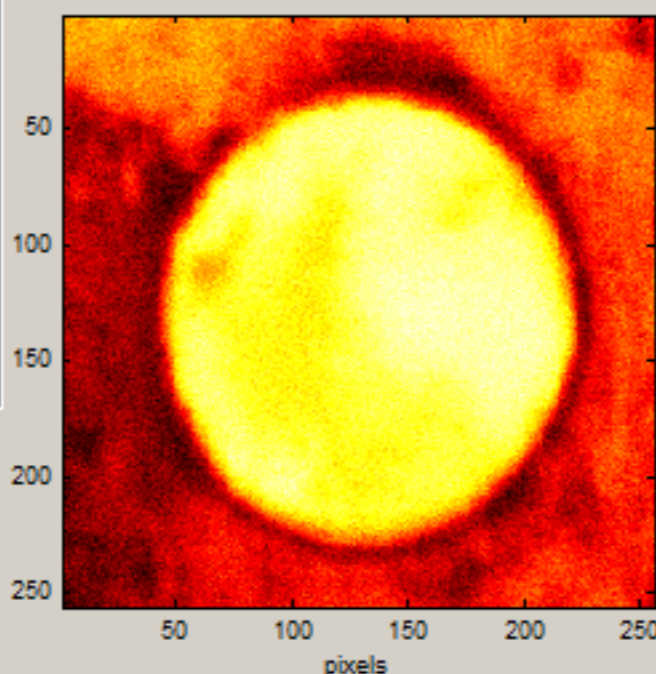
39.0251

39.9952

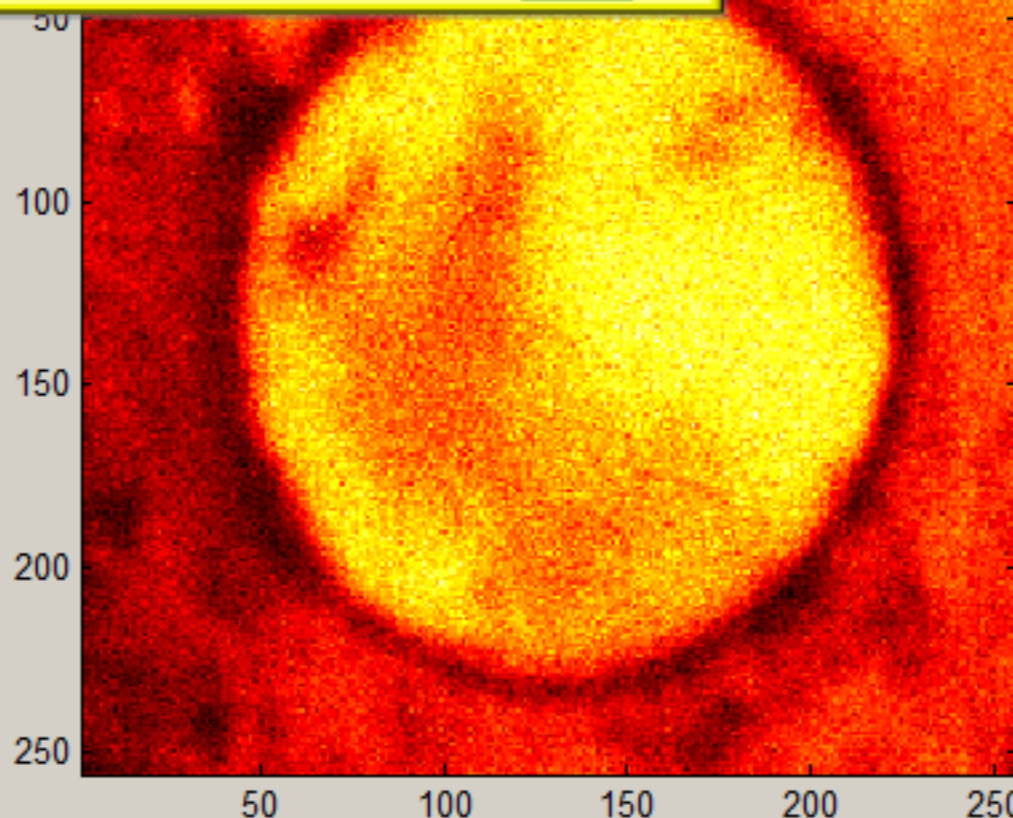
41.0043

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

Name of Image Matrix

Name of Variable Matrix

imagedata_PEG...

exactmass_PEGP...

Scores

Loadings

Variance

PCA_scores

PCA_loads

PCA_va

Load Selected Data

Image: imagedata_PEGPS_07

Variables: exactmass_PEGPS_07

Scores: PCA_scores

Loads: PCA_loads

Data Preprocessing

PoissonScaling & Mean C...

PC #

2

PCA Plot Options: Traditional

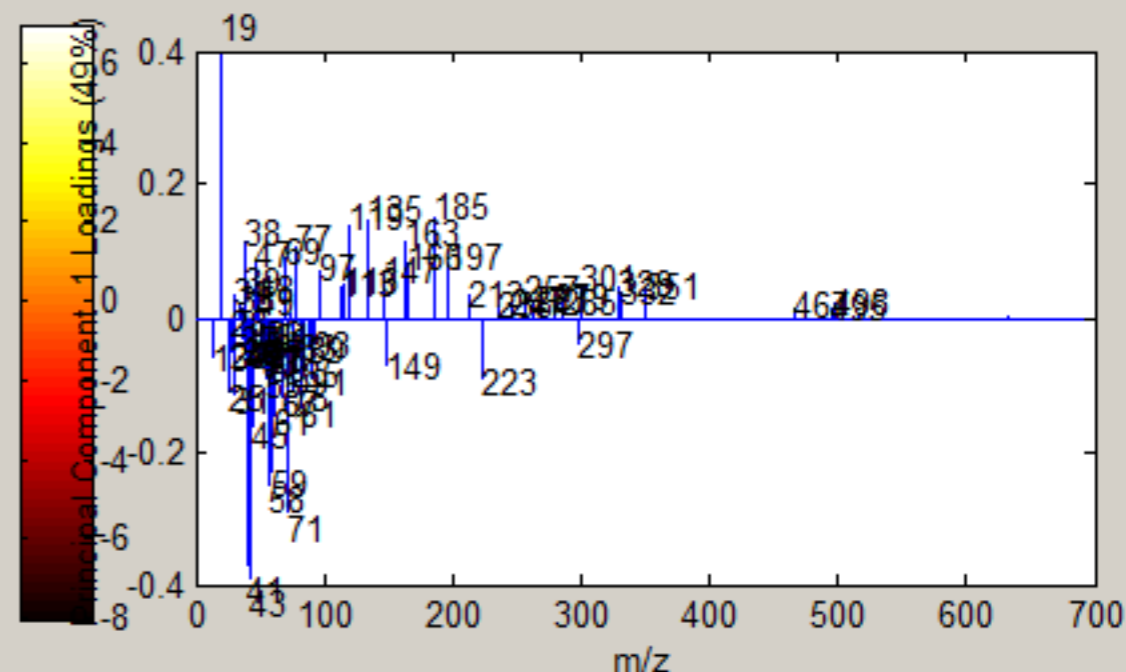
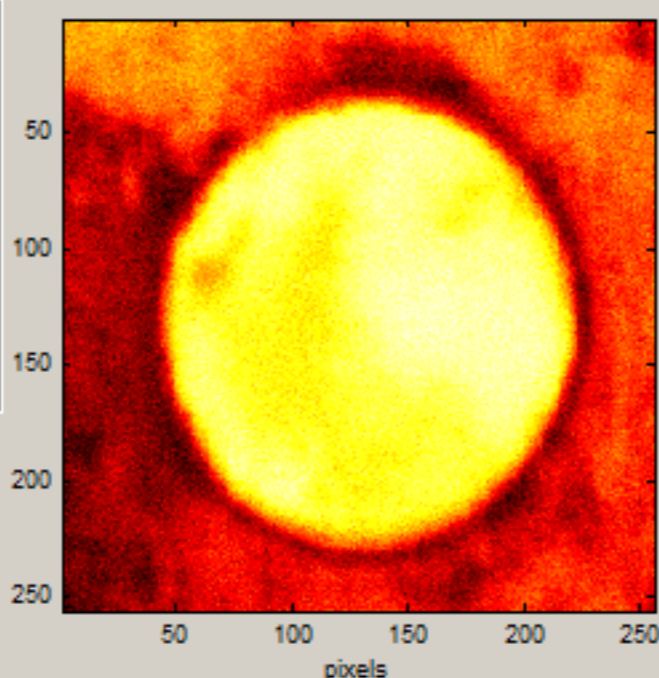
Plot Scores and Loads

Peak List

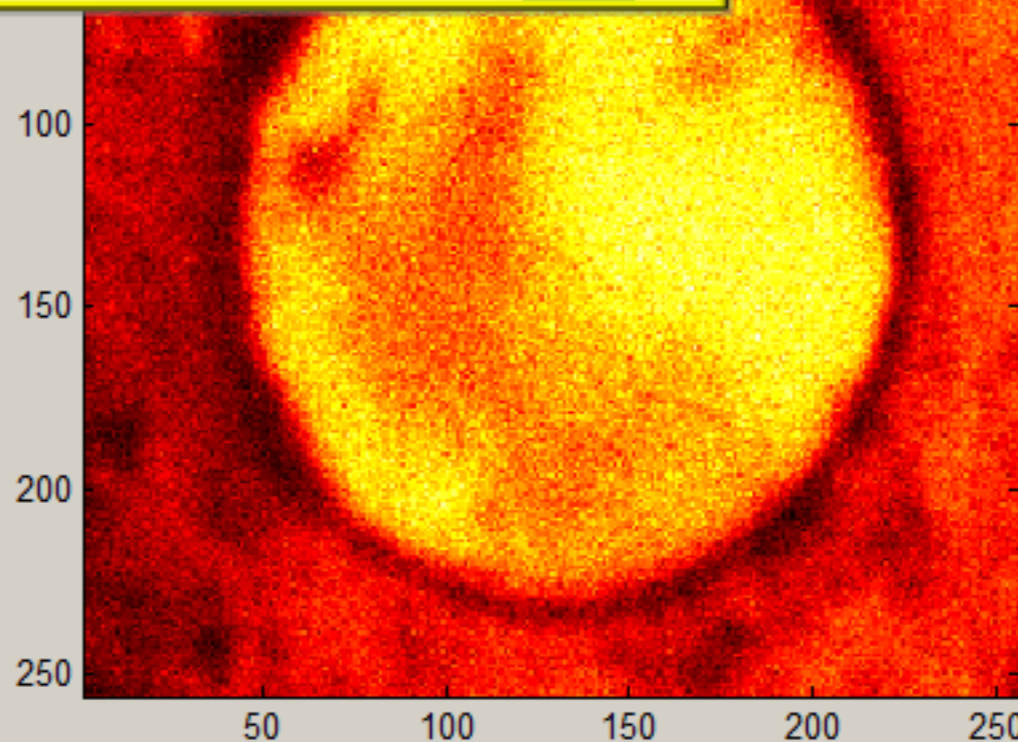
18.9985
25.0083
27.9764
29.0035
30.9976
31.0197
34.9697
34.9923
36.0001
37.0082
37.9961
38.0159
39.0052
39.0251
39.9952
41.0043

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

Name of Image Matrix

Name of Variable Matrix

imagedata_PEG...

exactmass_PEGP...

Scores

Loadings

Variance

PCA_scores

PCA_loads

PCA_va

Load Selected Data

Image: imagedata_PEGPS_07

Variables: exactmass_PEGPS_07

Scores: PCA_scores

Loads: PCA_loads

Data Preprocessing

PoissonScaling & Mean C...

PC #

2

PCA Plot Options: Traditional

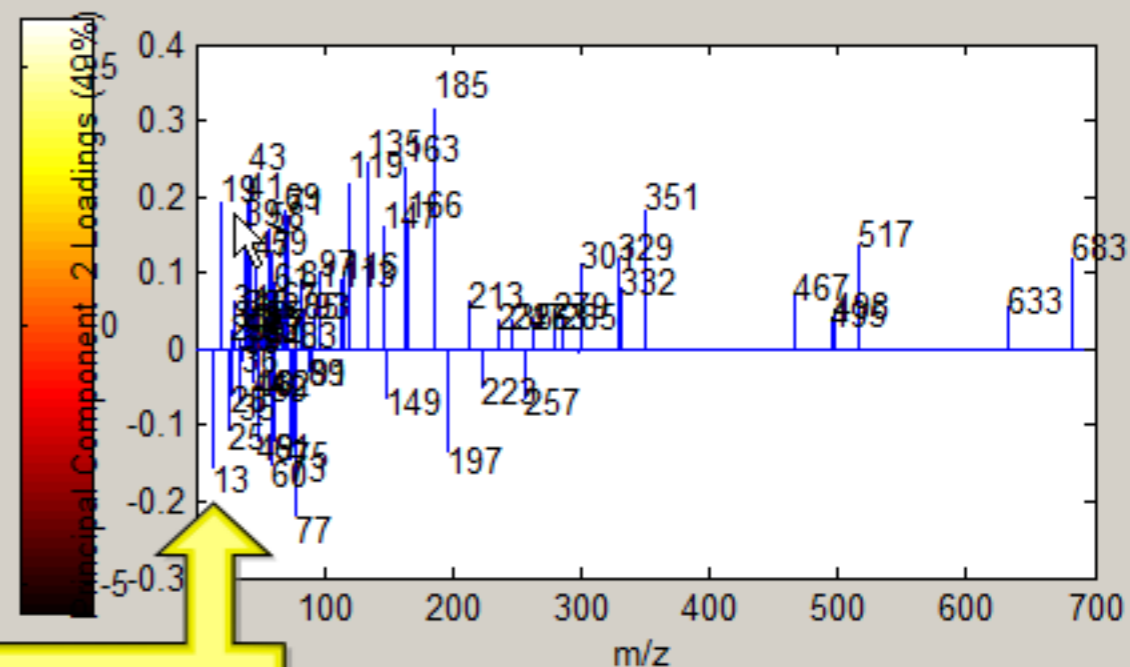
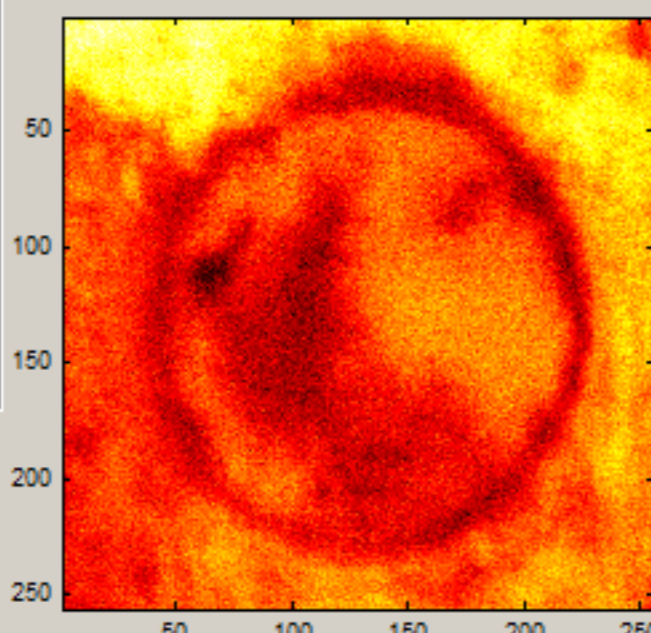
Plot Scores and Loads

Peak List

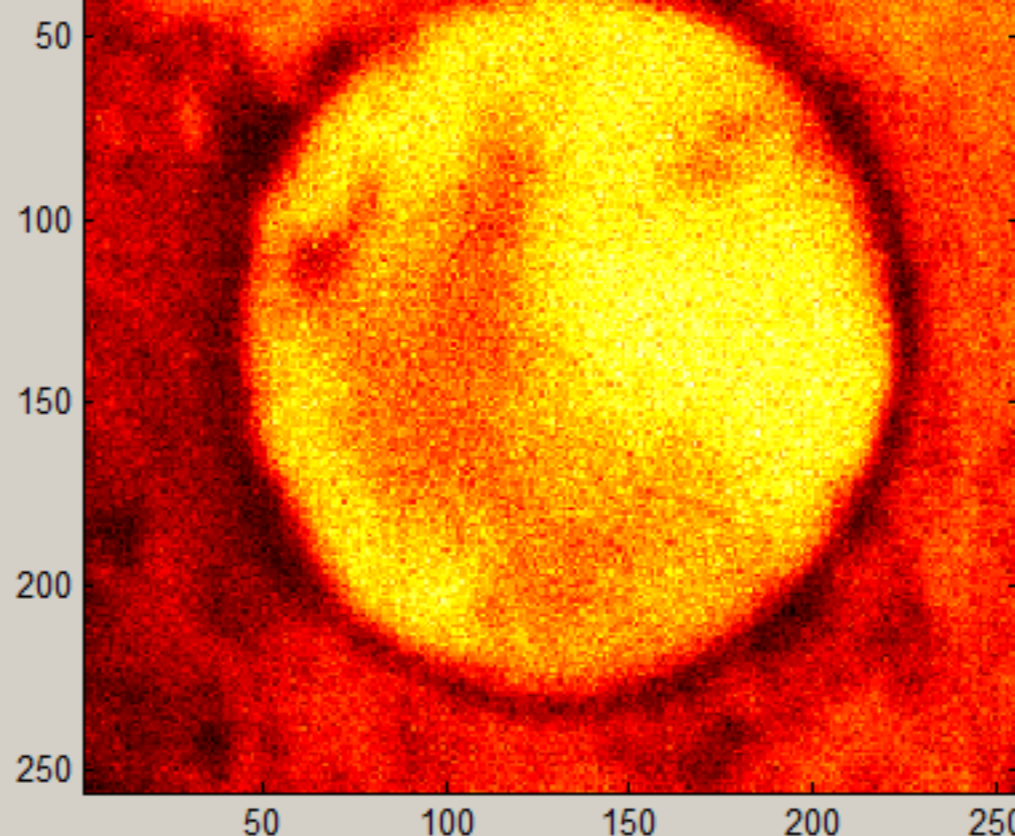
18.9985
25.0083
27.9764
29.0035
30.9976
31.0197
34.9697
34.9923
36.0001
37.0082
37.9961
38.0159
39.0052
39.0251
39.9952
41.0043

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 19 peak shows a positive loading on PC2, but it no longer has the highest loading.



Save Figure

Make Ext

Close Panel

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

imagedata_PEG...

exactmass_PEGP...

Scores

Loadings

Variance

PCA_scores

PCA_loads

PCA_va

Load Selected Data

Image: imagedata_PEGPS_07

Variables: exactmass_PEGPS_07

Scores: PCA_scores

Loads: PCA_loads

Data Preprocessing

PoissonScaling & Mean C...

PC #

2

PCA Plot Options: Traditional

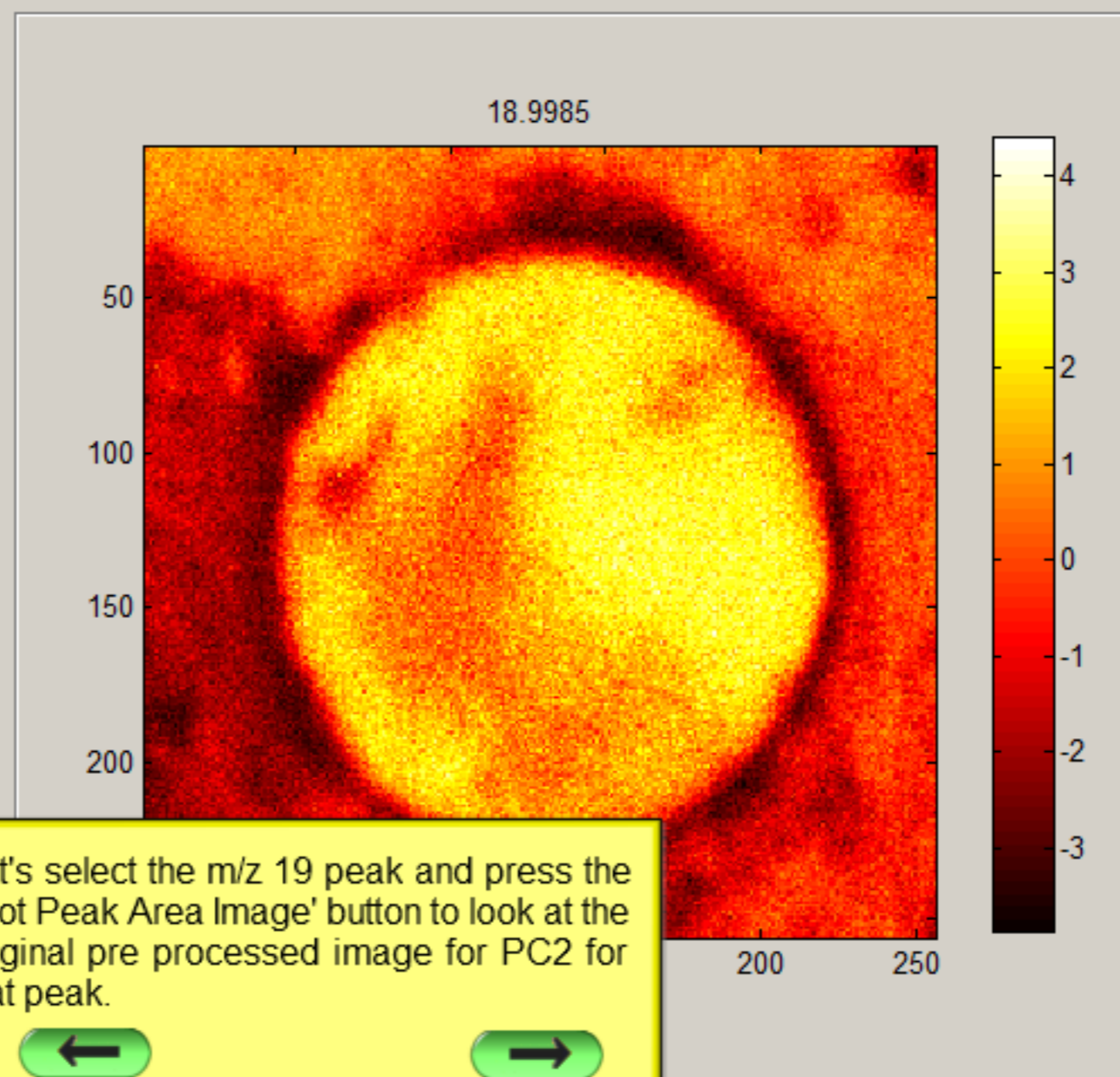
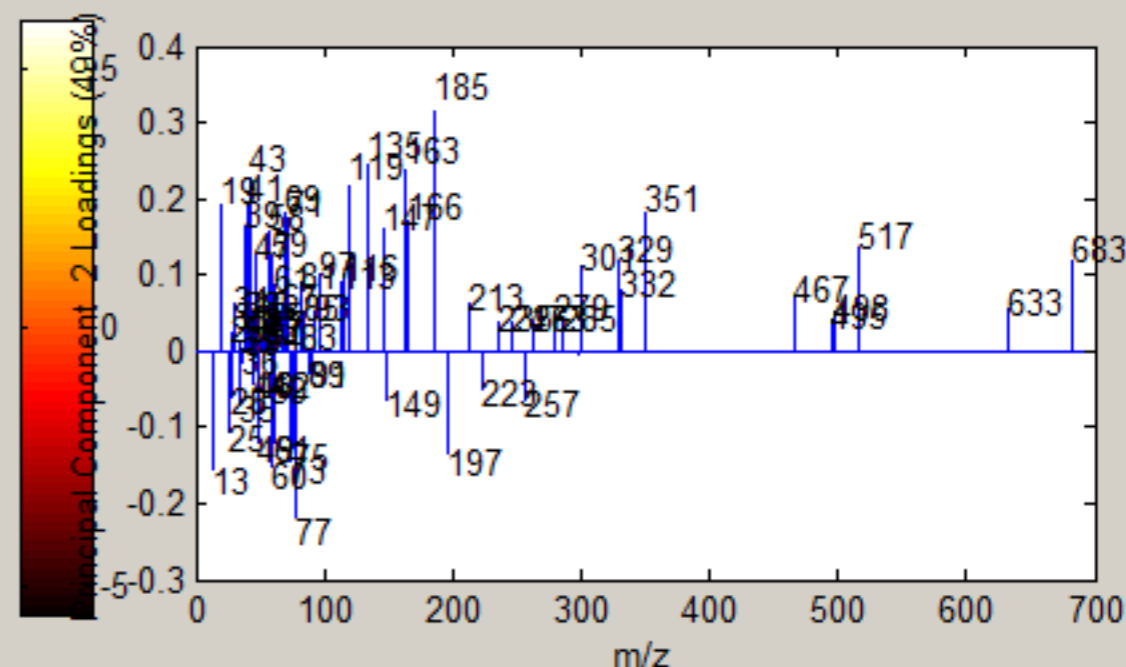
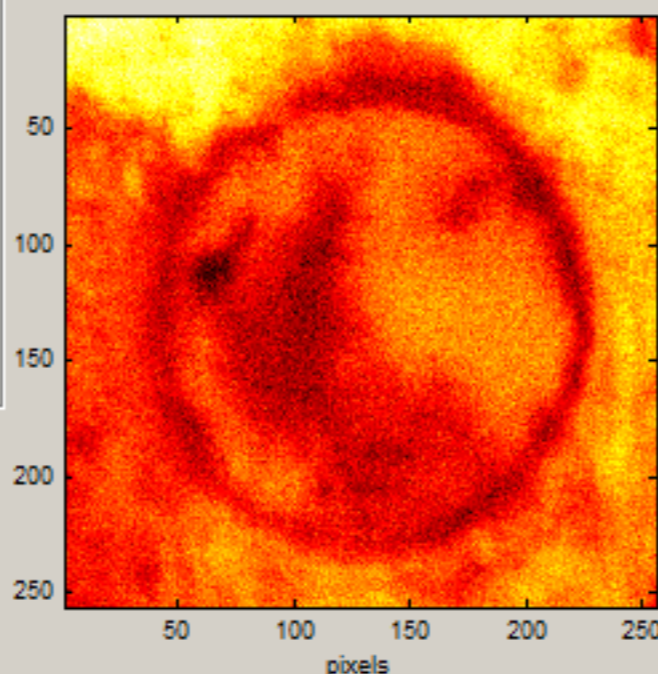
Plot Scores and Loads

Peak List

18.9985
25.0083
27.9764
29.0035
30.9976
31.0197
34.9697
34.9923
36.0001
37.0082
37.9961
38.0159
39.0052
39.0251
39.9952
41.0043

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 19 peak and press the
'Plot Peak Area Image' button to look at the
original pre processed image for PC2 for
that peak.



Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

imagedata_PEG...

exactmass_PEGP...

Scores

Loadings

Variance

PCA_scores

PCA_loads

PCA_va

Load Selected Data

Image: imagedata_PEGPS_07

Variables: exactmass_PEGPS_07

Scores: PCA_scores

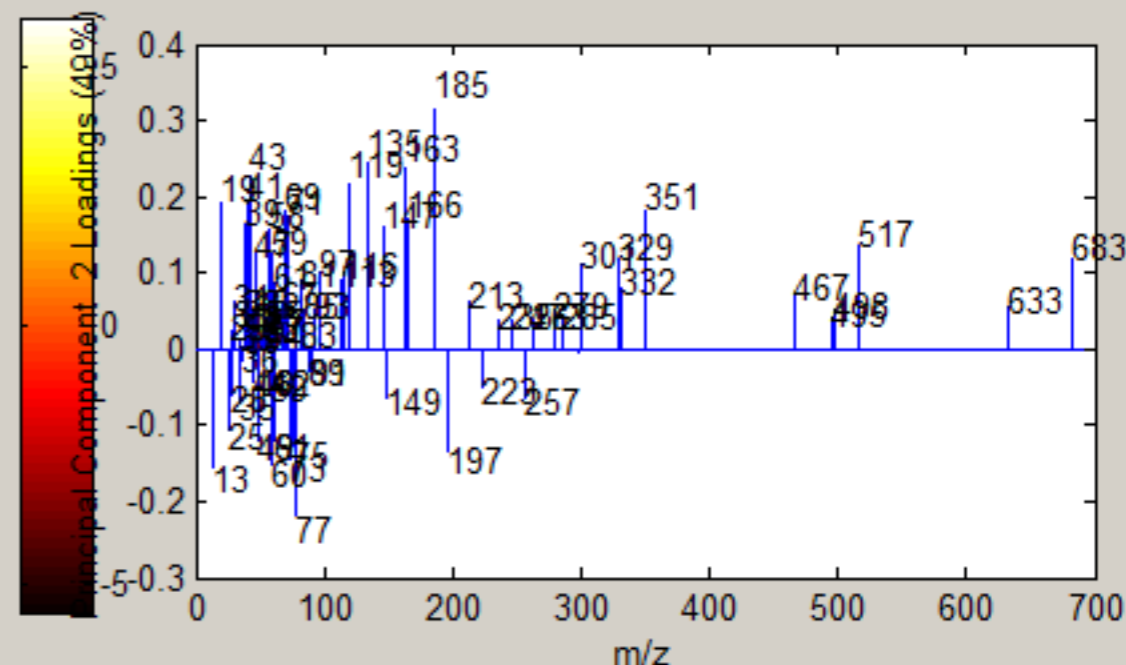
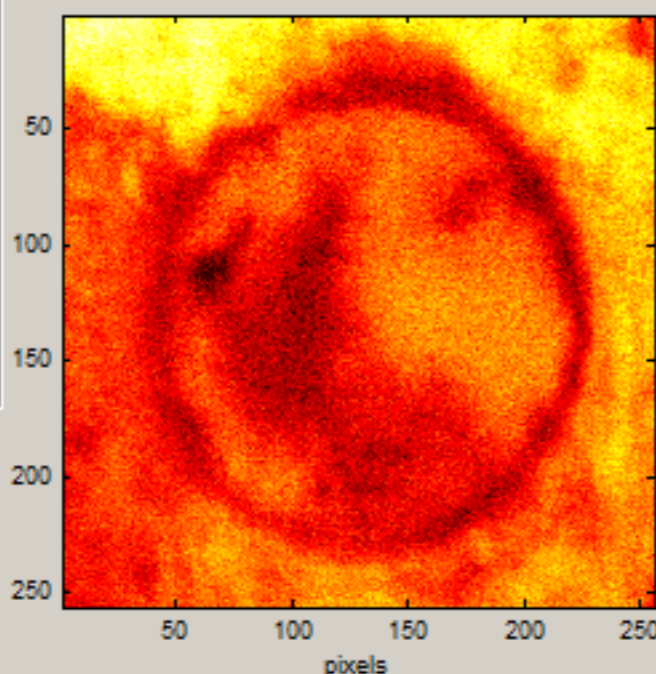
Loads: PCA_loads

Data Preprocessing

PoissonScaling & Mean C...

PC #

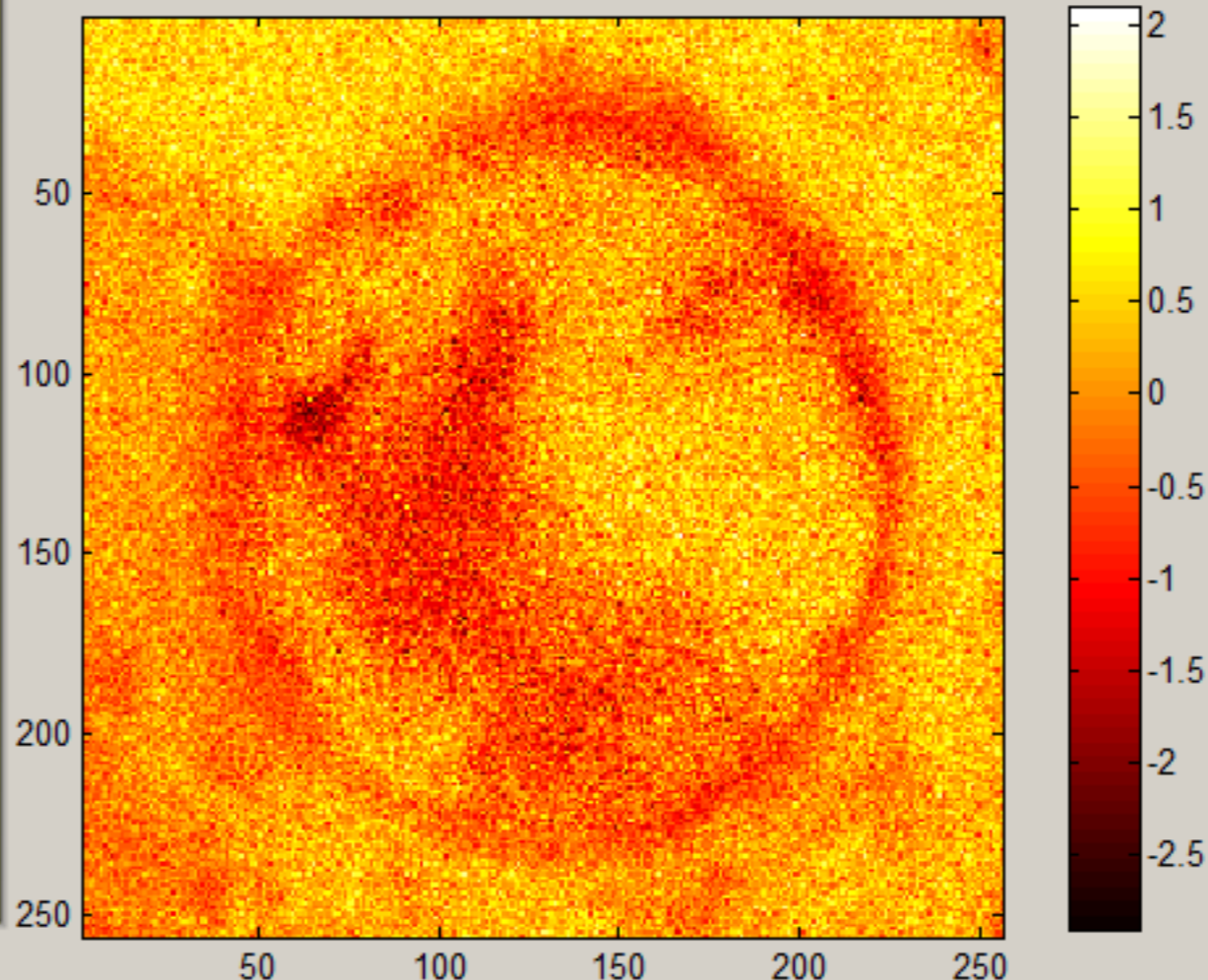
2



Here we see the pre processed image data for the m/z 19 peak after subtracting PC1 from the data set. The general pattern is similar to that seen in the PC2 scores image, and it is very different from that seen before subtracting PC1 from the data set.

This image makes more sense than the image from the pre processed data before subtracting PC1 for understanding what is happening in PC2. Before subtracting PC1 the m/z 19 peak area image mainly showed signal on the spot, however PC2 shows higher scores in the upper right corner and somewhat on the spot. This is consistent with the data shown after subtracting PC1.

18.9985



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

Name of Image Matrix

Name of Variable Matrix

imagedata_PEG...

exactmass_PEGP...

Scores

Loadings

Variance

PCA_scores

PCA_loads

PCA_va

Load Selected Data

Image: imagedata_PEGPS_07

Variables: exactmass_PEGPS_07

Scores: PCA_scores

Loads: PCA_loads

Data Preprocessing

PoissonScaling & Mean C...

PC #

1

PCA Plot Options: Traditional

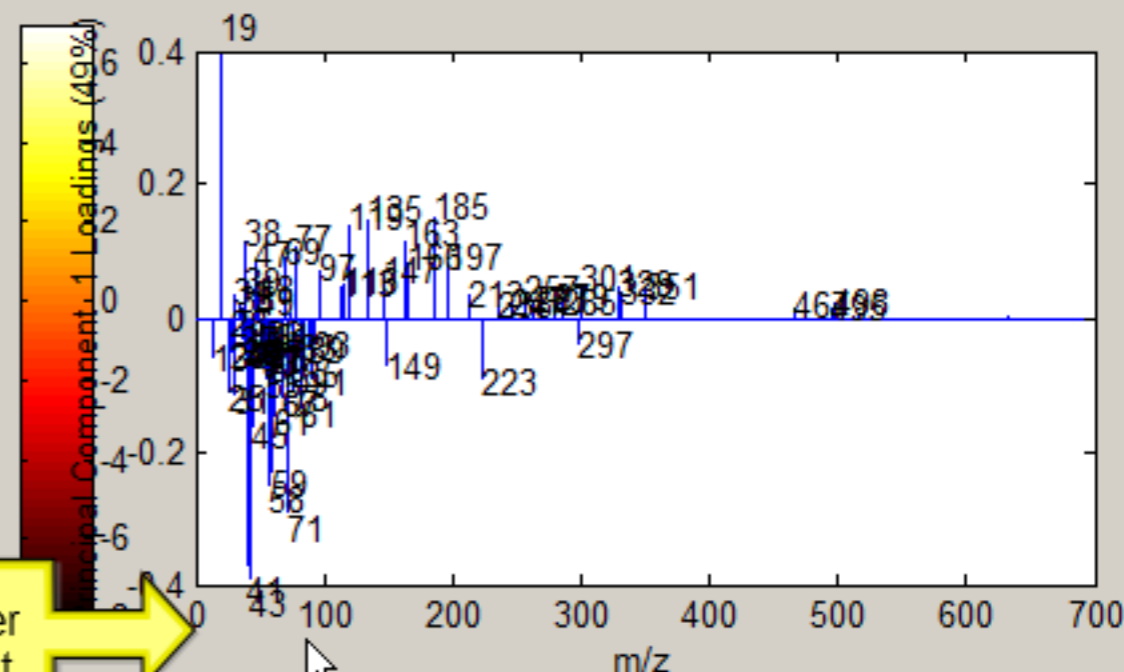
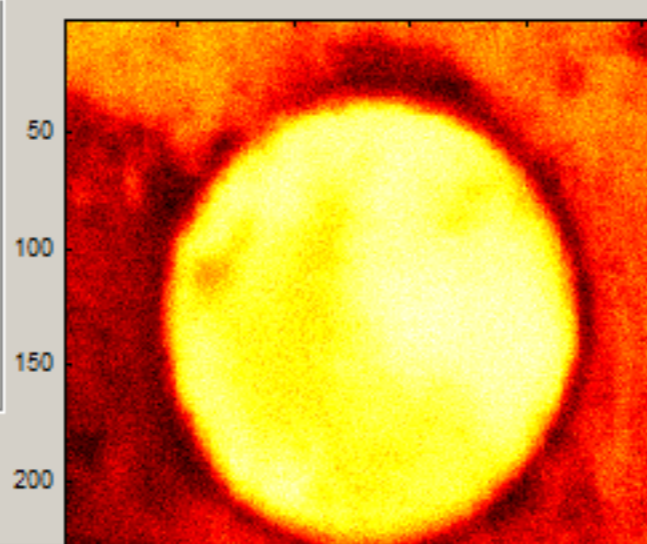
Plot Scores and Loads

Peak List

13.0086
18.9985
25.0083
27.9764
29.0035
30.9976
31.0197
34.9697
34.9923
36.0001
37.0082
37.9961
38.0159
39.0052
39.0251
39.9952

Plot Peak Area Image

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



Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

PCA_scores

Loadings

PCA_loads

Variance

PCA_va

Load Selected Data

Image: imagedata_PEGPS_07

Variables: exactmass_PEGPS_07

Scores: PCA_scores

Loads: PCA_loads

Data Preprocessing

PoissonScaling & Mean C...

PC #

1

PCA Plot Options: Traditional

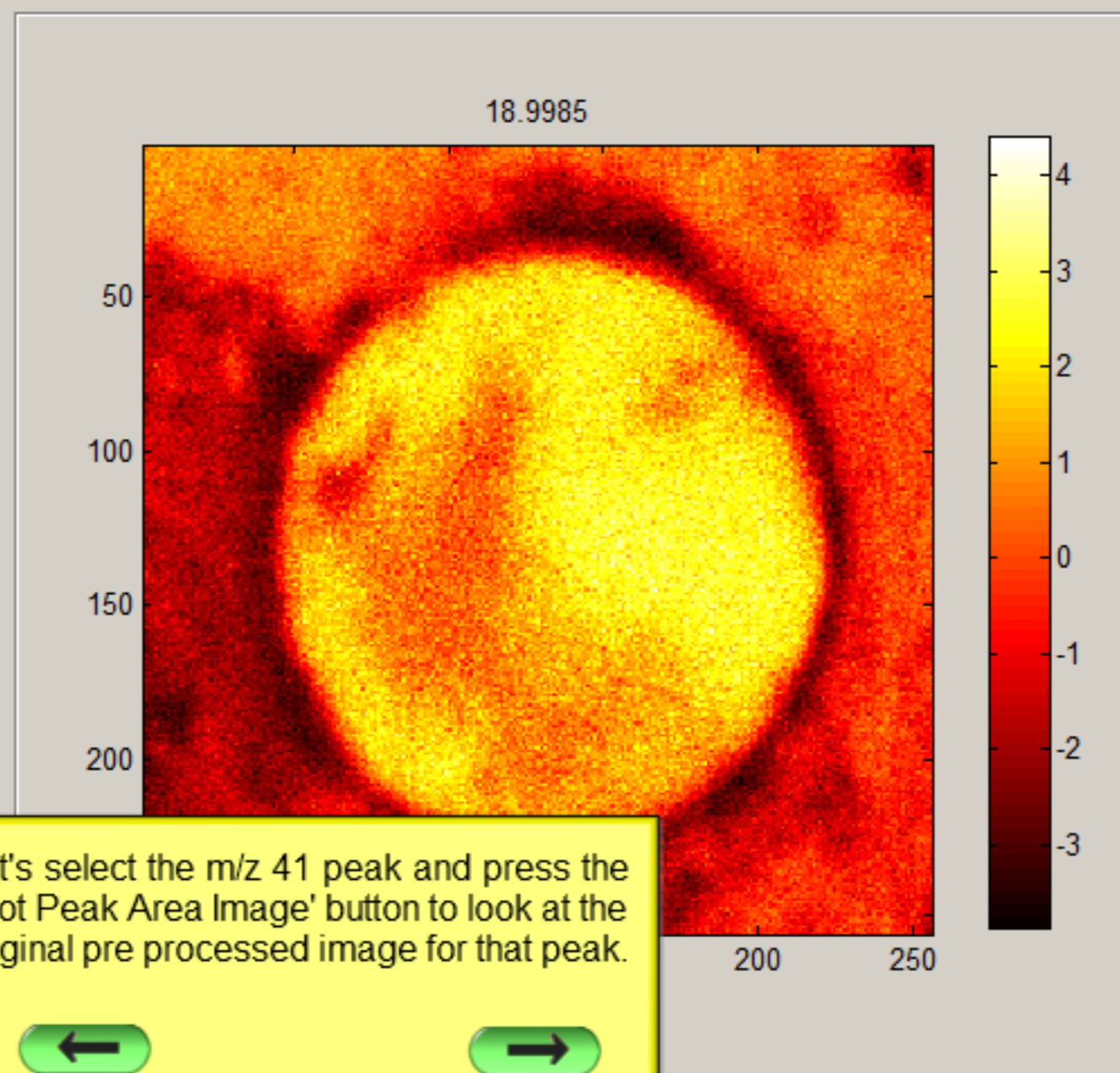
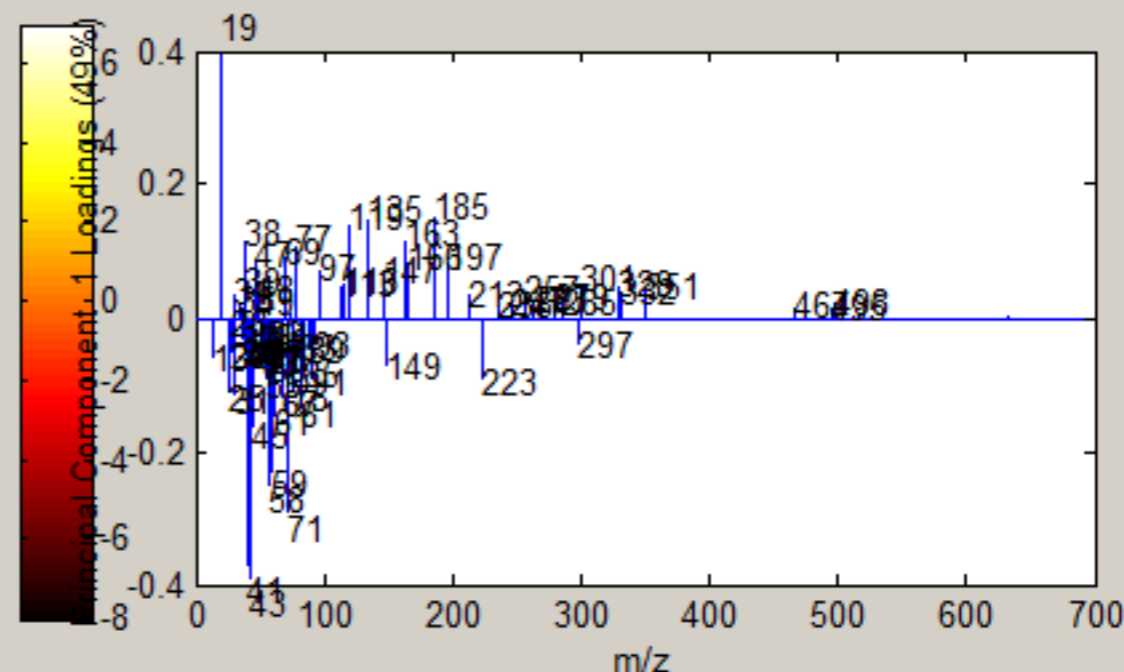
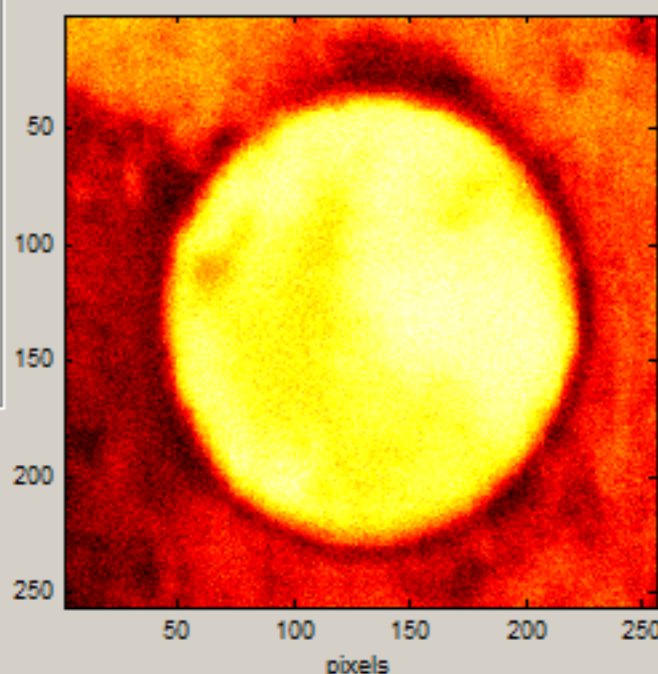
Plot Scores and Loads

Peak List

25.0083
27.9764
29.0035
30.9976
31.0197
34.9697
34.9923
36.0001
37.0082
37.9961
38.0159
39.0052
39.0251
39.9952
41.0043
42.0081

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 41 peak and press the 'Plot Peak Area Image' button to look at the original pre processed image for that peak.



Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

imagedata_PEG...

exactmass_PEGP...

Scores

Loadings

Variance

PCA_scores

PCA_loads

PCA_va

Load Selected Data

Image: imagedata_PEGPS_07

Variables: exactmass_PEGPS_07

Scores: PCA_scores

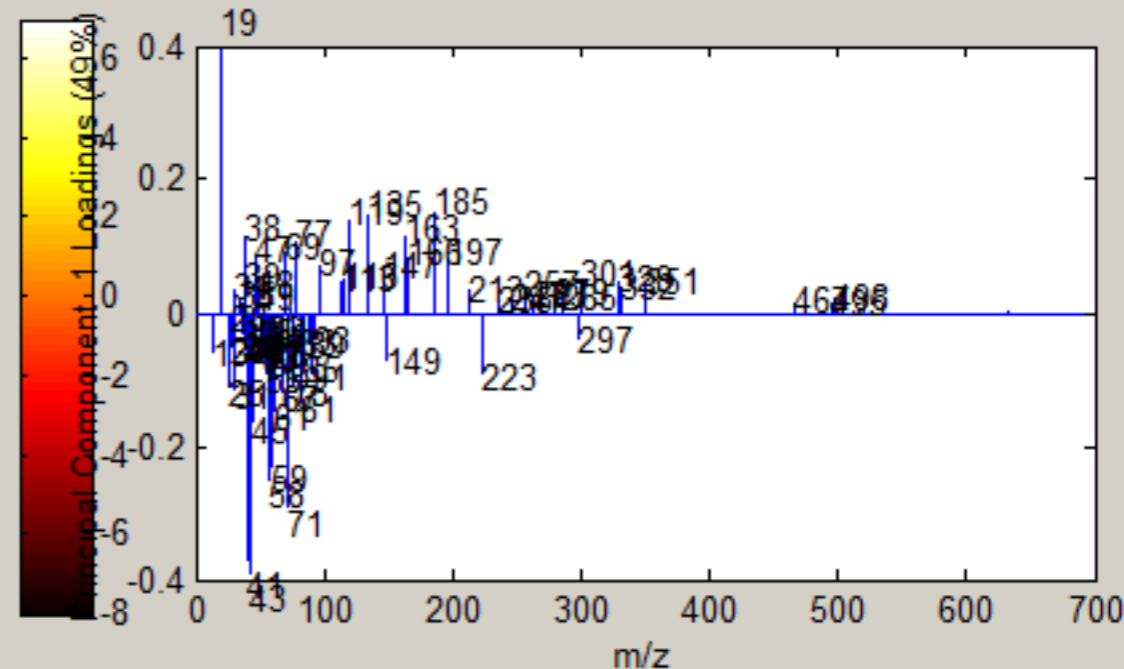
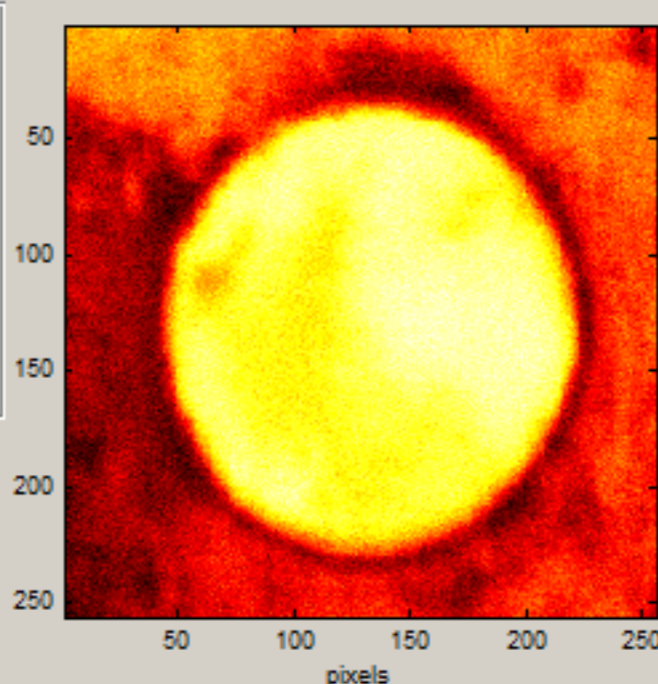
Loads: PCA_loads

Data Preprocessing

PoissonScaling & Mean C...

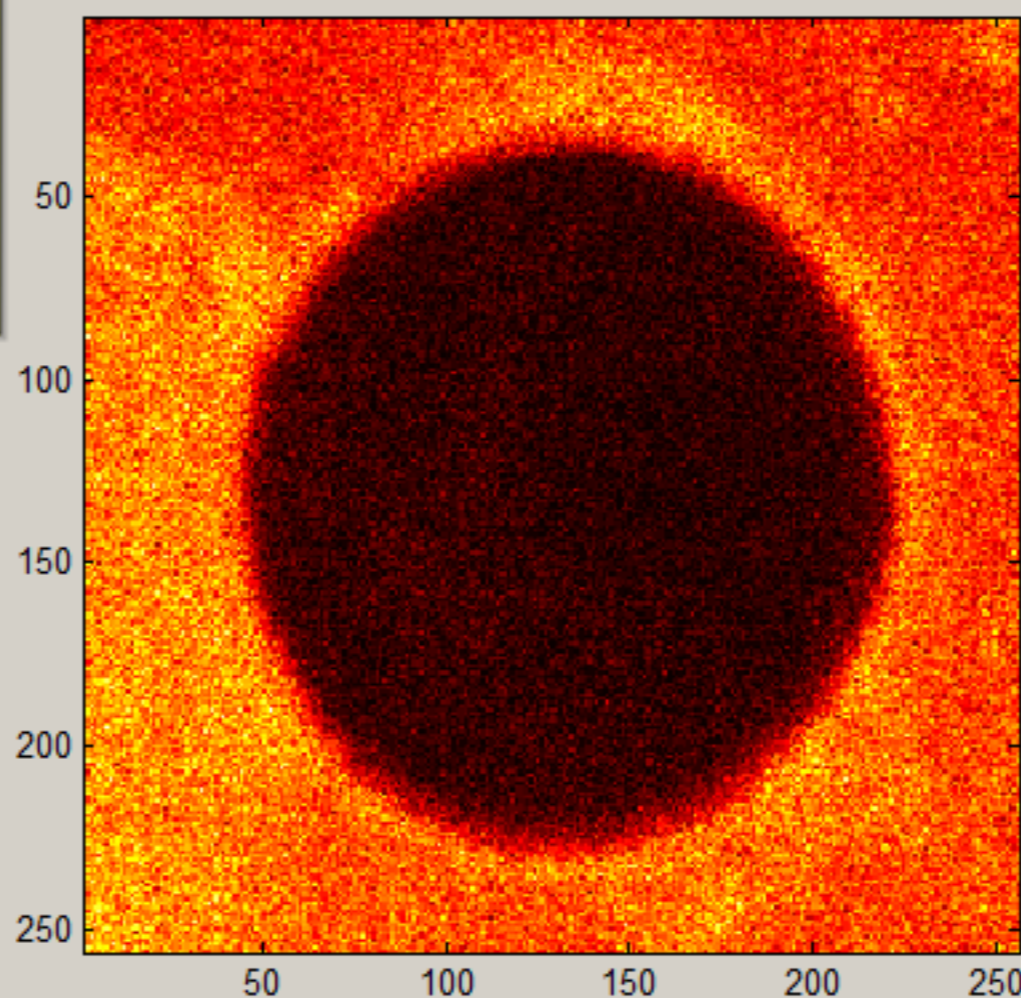
PC #

1



As expected the peak area image shows a trend very similar to that seen in the PC1 scores image. The m/z 41 peak shows a higher relative intensity outside of the spot with the highest relative intensity in the bottom left corner.

41.0043



Save Figure

Make Ext

Close Panel

31.0197
34.9697
34.9923
36.0001
37.0082
37.9961
38.0159
39.0052
39.0251
39.9952
41.0043
42.0081

Plot Peak Area Image

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

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

imagedata_PEG...

exactmass_PEGP...

Scores

Loadings

Variance

PCA_scores

PCA_loads

PCA_va

Load Selected Data

Image: imagedata_PEGPS_07

Variables: exactmass_PEGPS_07

Scores: PCA_scores

Loads: PCA_loads

Data Preprocessing

PoissonScaling & Mean C...

PC #

2

PCA Plot Options: Traditional

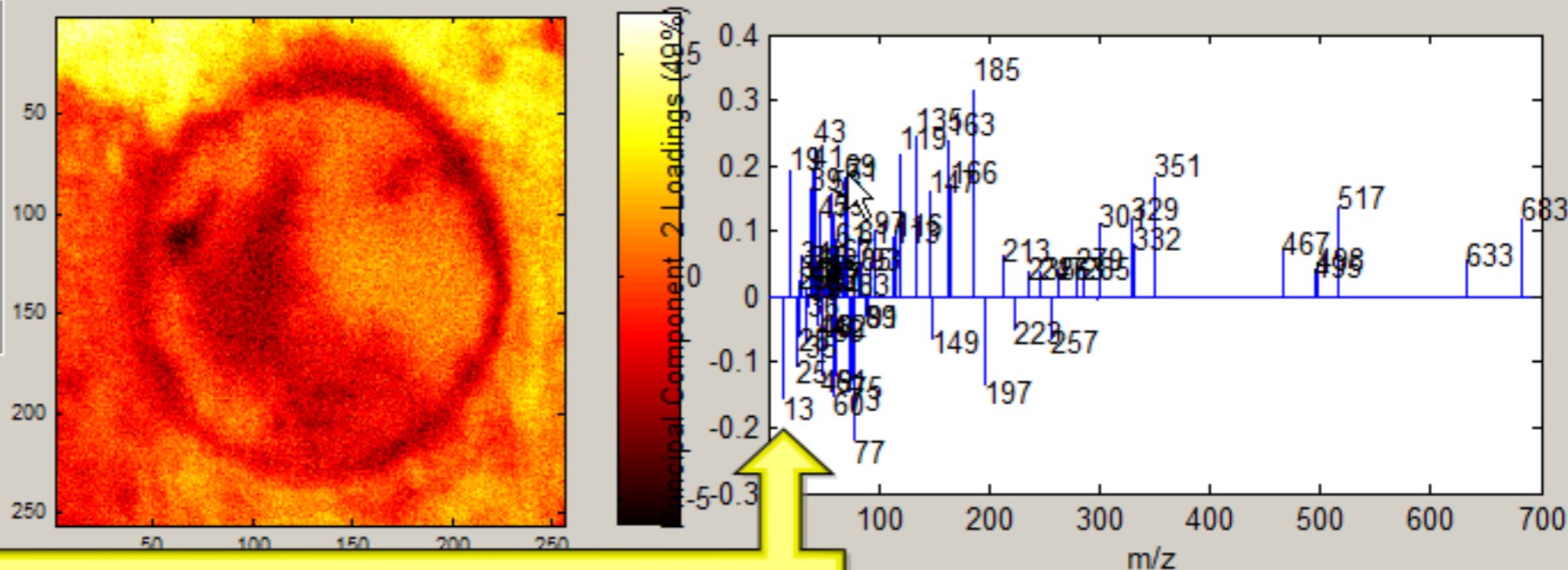
Plot Scores and Loads

Peak List

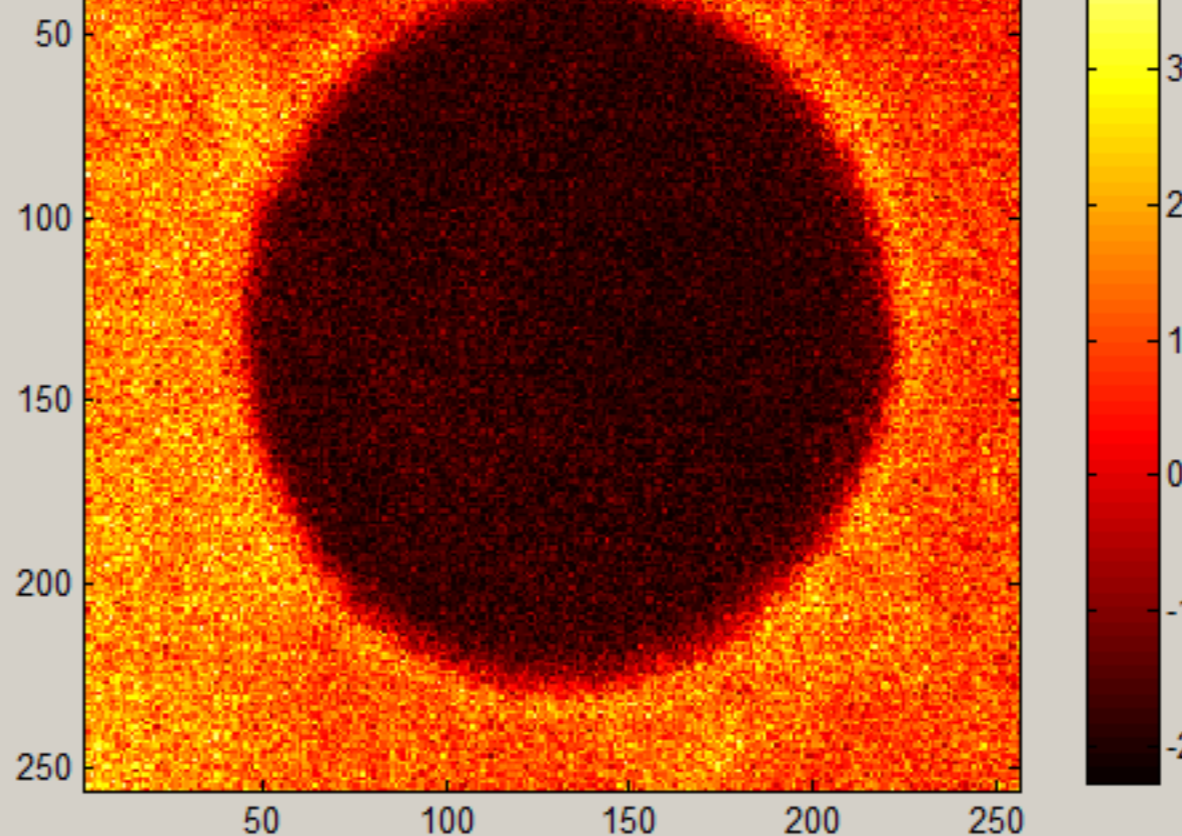
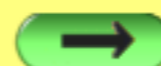
25.0083
27.9764
29.0035
30.9976
31.0197
34.9697
34.9923
36.0001
37.0082
37.9961
38.0159
39.0052
39.0251
39.9952
41.0043
42.0081

Plot Peak Area Image

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



Now let's look at PC2. On PC2 the m/z 41 peak shows a positive loading. We would then expect that it shows a higher relative intensity in the upper right corner and somewhat on the spot.



Save Figure

Make Ext

Close Panel

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

imagedata_PEG...

exactmass_PEGP...

Scores

Loadings

Variance

PCA_scores

PCA_loads

PCA_va

Load Selected Data

Image: imagedata_PEGPS_07

Variables: exactmass_PEGPS_07

Scores: PCA_scores

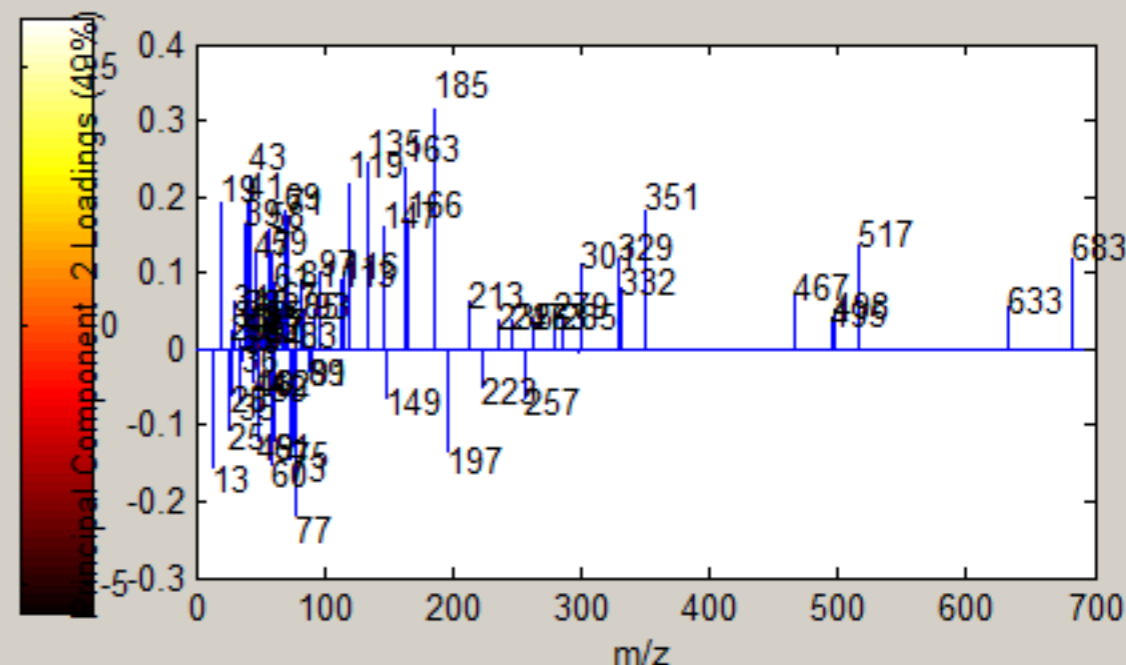
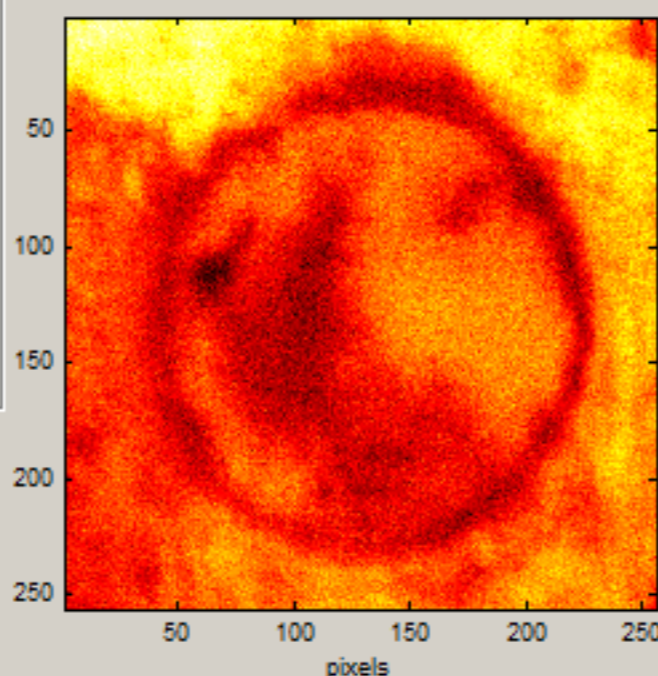
Loads: PCA_loads

Data Preprocessing

PoissonScaling & Mean C...

PC #

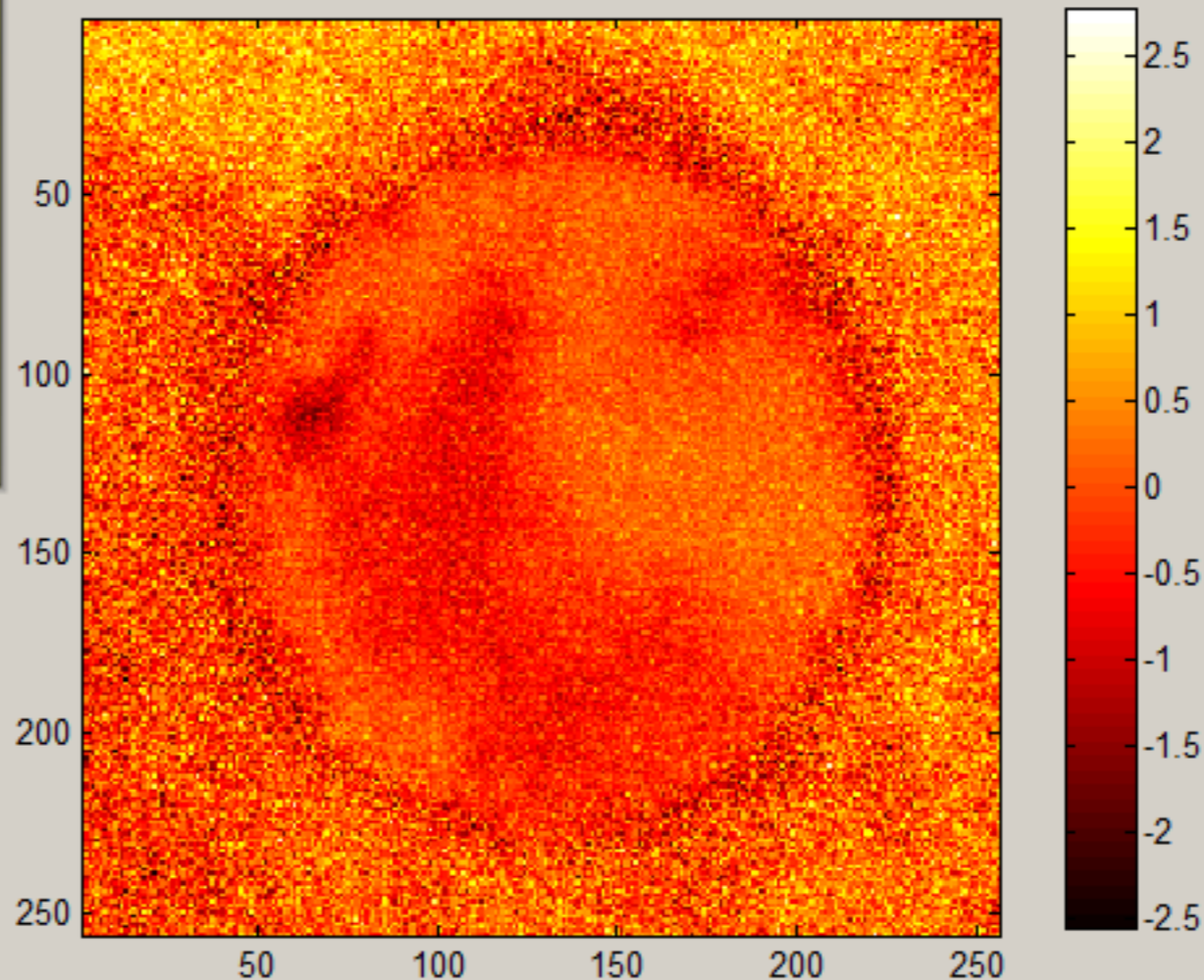
2



Here we see the pre processed image data for the m/z 41 peak after subtracting PC1 from the data set. The image looks as expected with a higher relative intensity in the upper right corner and some signal on the spot and below.

Once again using the subtracted data allows us to see the trends in the data that PCA was capturing.

41.0043



Save Figure

Make Ext

Close Panel

37.0082
37.9961
38.0159
39.0052
39.0251
39.9952
41.0043
42.0081

Plot Peak Area Image

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

Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

PCA_scores

Loadings

PCA_loads

Variance

PCA_va

Load Selected Data

Image: imagedata_PEGPS_07

Variables: exactmass_PEGPS_07

Scores: PCA_scores

Loads: PCA_loads

Data Preprocessing

PoissonScaling & Mean C...

PC #

2

PCA Plot Options: Traditional

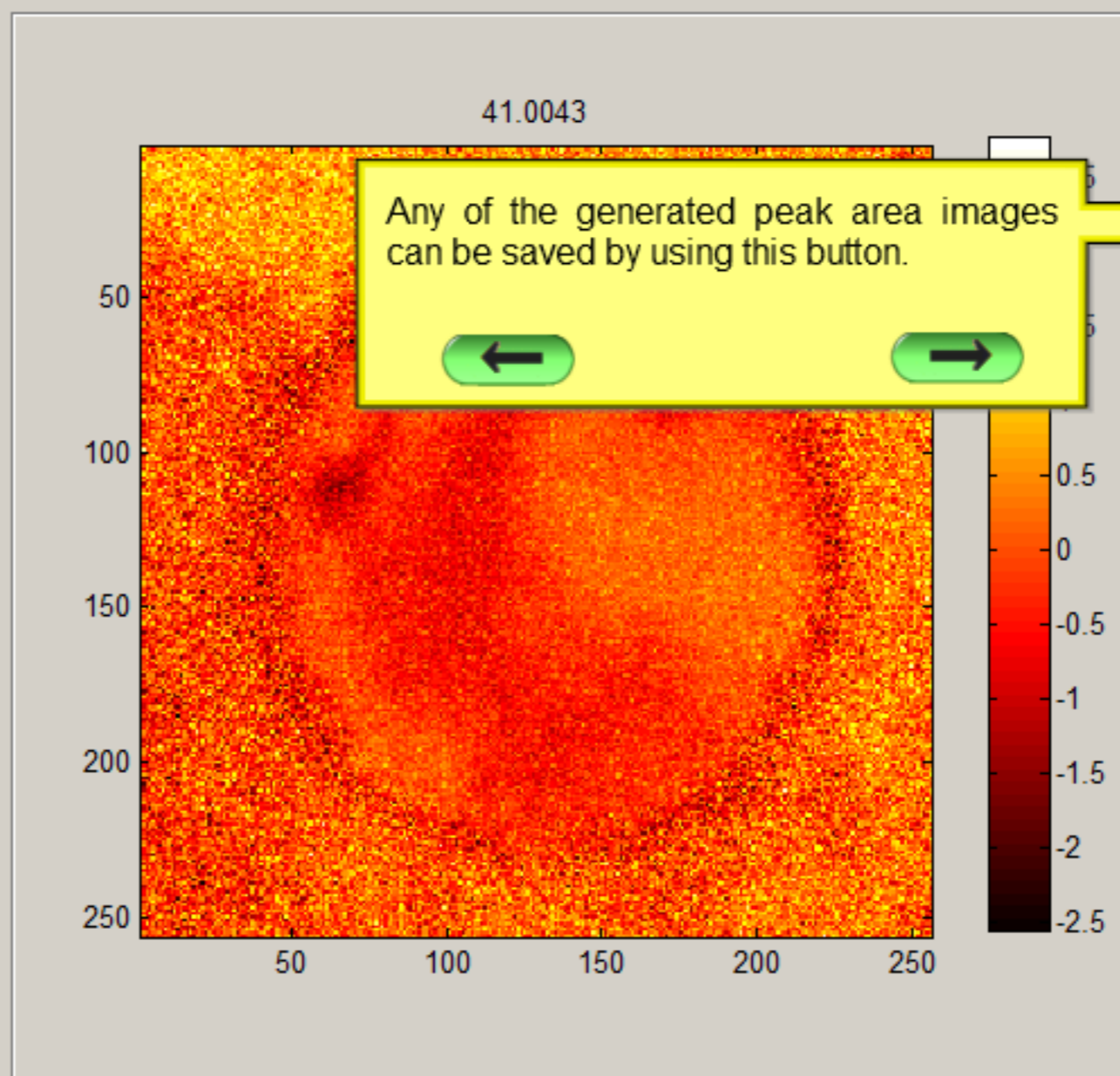
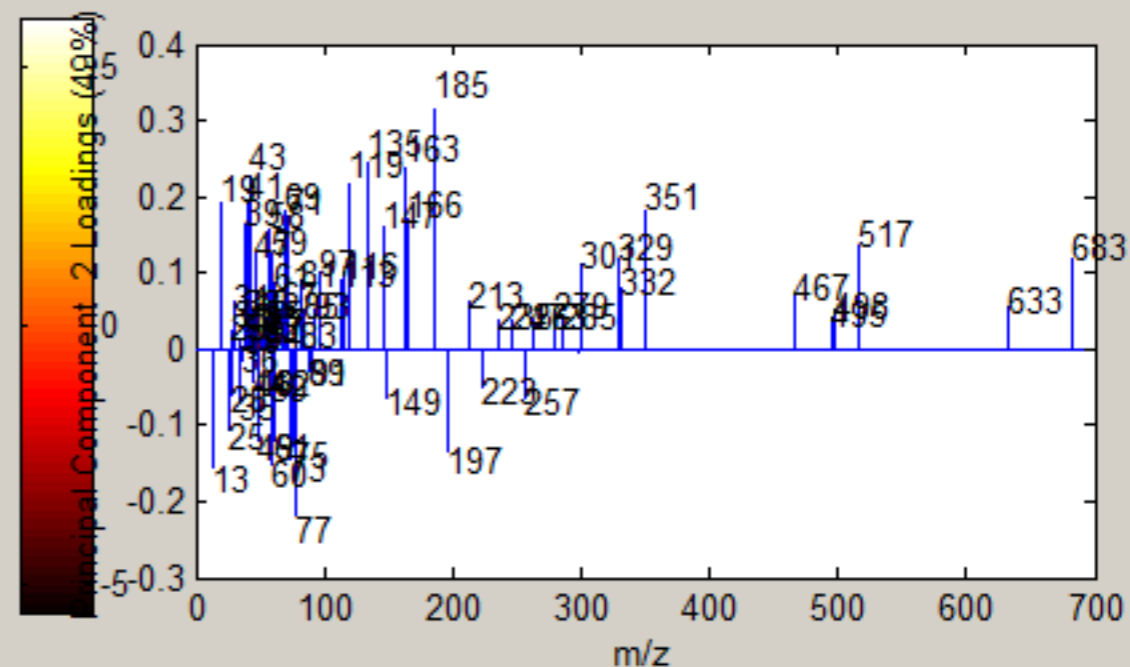
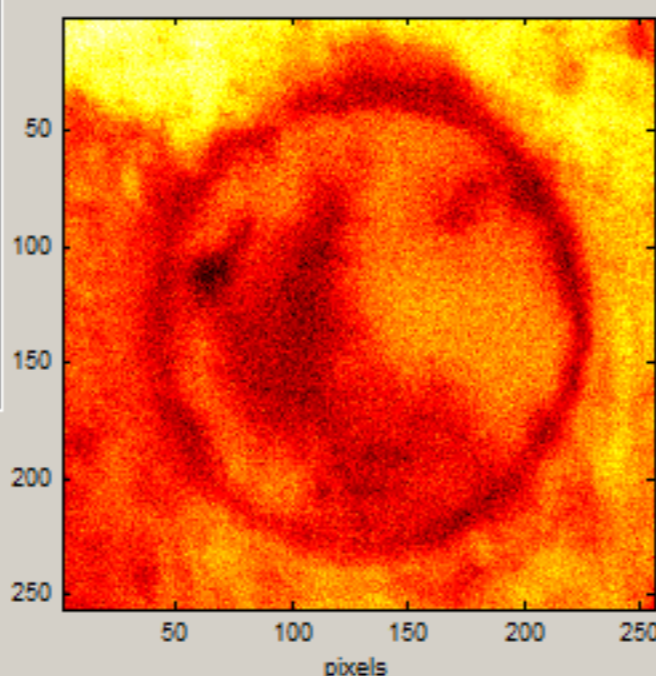
Plot Scores and Loads

Peak List

25.0083
27.9764
29.0035
30.9976
31.0197
34.9697
34.9923
36.0001
37.0082
37.9961
38.0159
39.0052
39.0251
39.9952
41.0043
42.0081

Plot Peak Area Image

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



Any of the generated peak area images
can be saved by using this button.

Save Figure

Make Ext

Close Panel

Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

PCA_scores

Loadings

PCA_loads

Variance

PCA_va

Load Selected Data

Image: imagedata_PEGPS_07

Variables: exactmass_PEGPS_07

Scores: PCA_scores

Loads: PCA_loads

Data Preprocessing

PoissonScaling & Mean C...

PC #

2

PCA Plot Options: Traditional

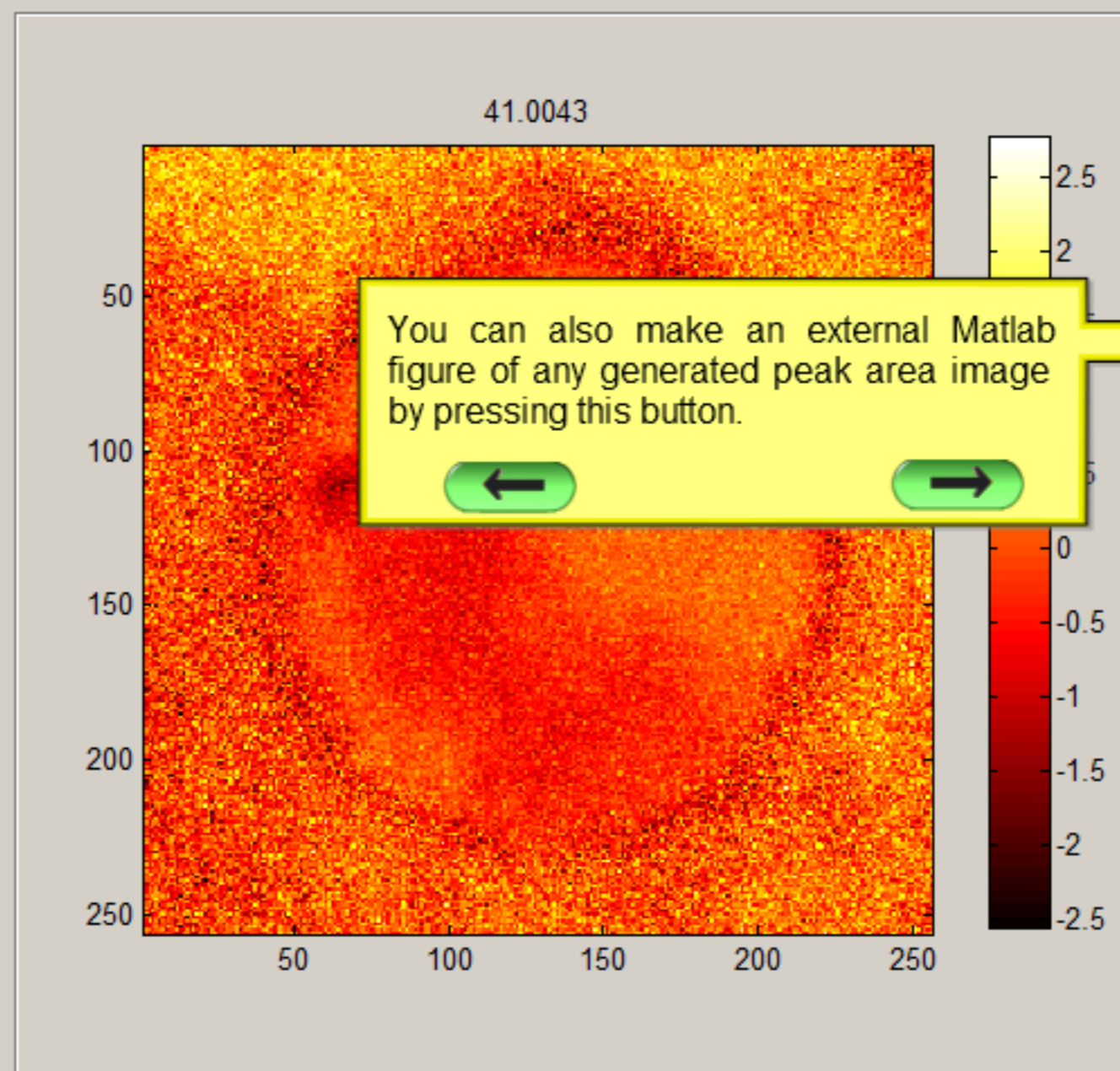
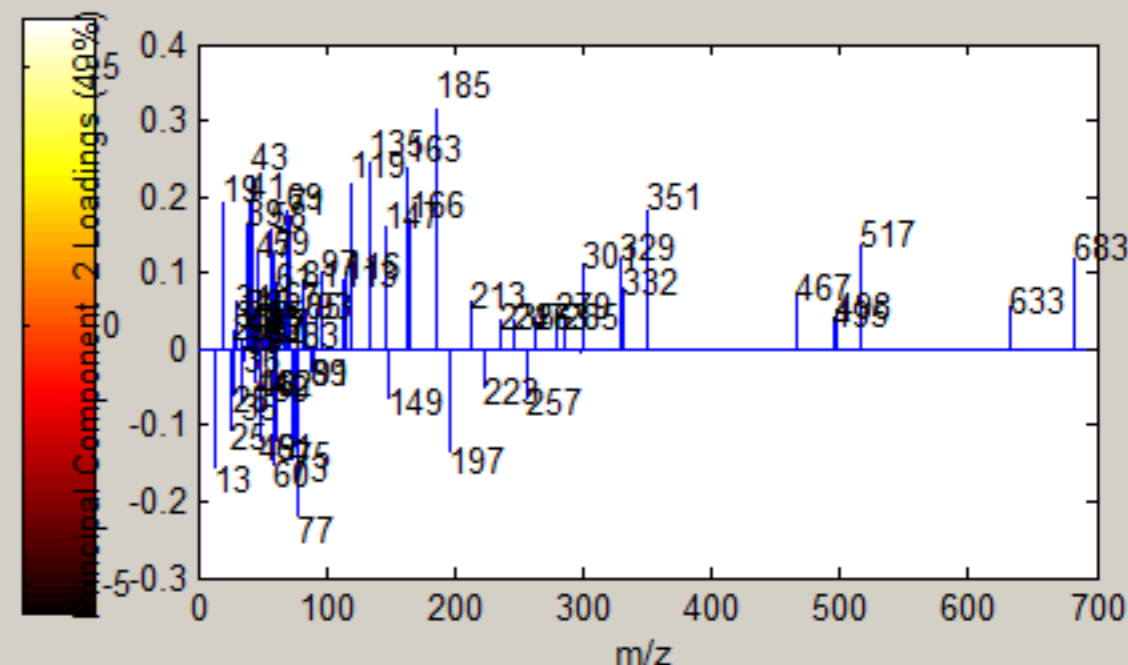
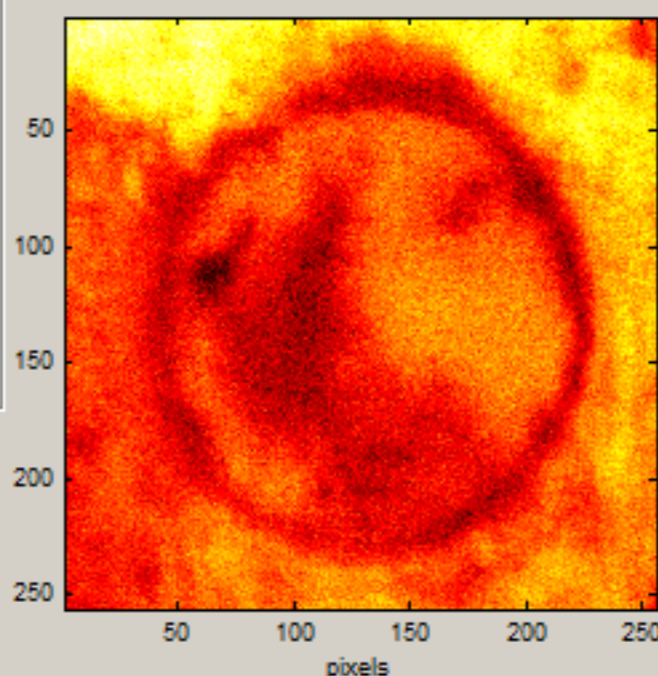
Plot Scores and Loads

Peak List

25.0083
27.9764
29.0035
30.9976
31.0197
34.9697
34.9923
36.0001
37.0082
37.9961
38.0159
39.0052
39.0251
39.9952
41.0043
42.0081

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

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

PCA_scores

Loadings

PCA_loads

Variance

PCA_va

Load Selected Data

Image: imagedata_PEGPS_07

Variables: exactmass_PEGPS_07

Scores: PCA_scores

Loads: PCA_loads

Data Preprocessing

PoissonScaling & Mean C...

PC #

2

PCA Plot Options: Traditional

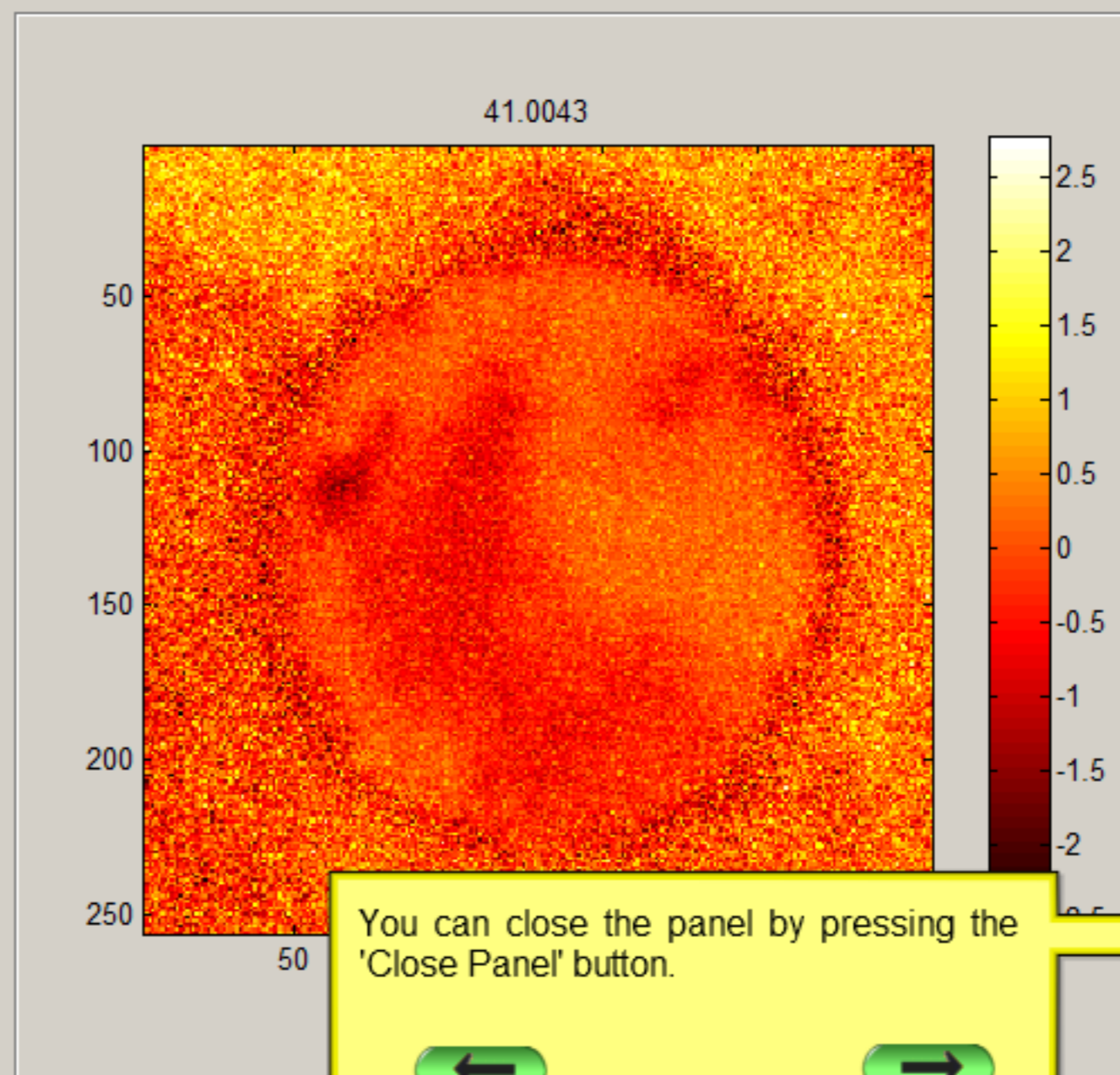
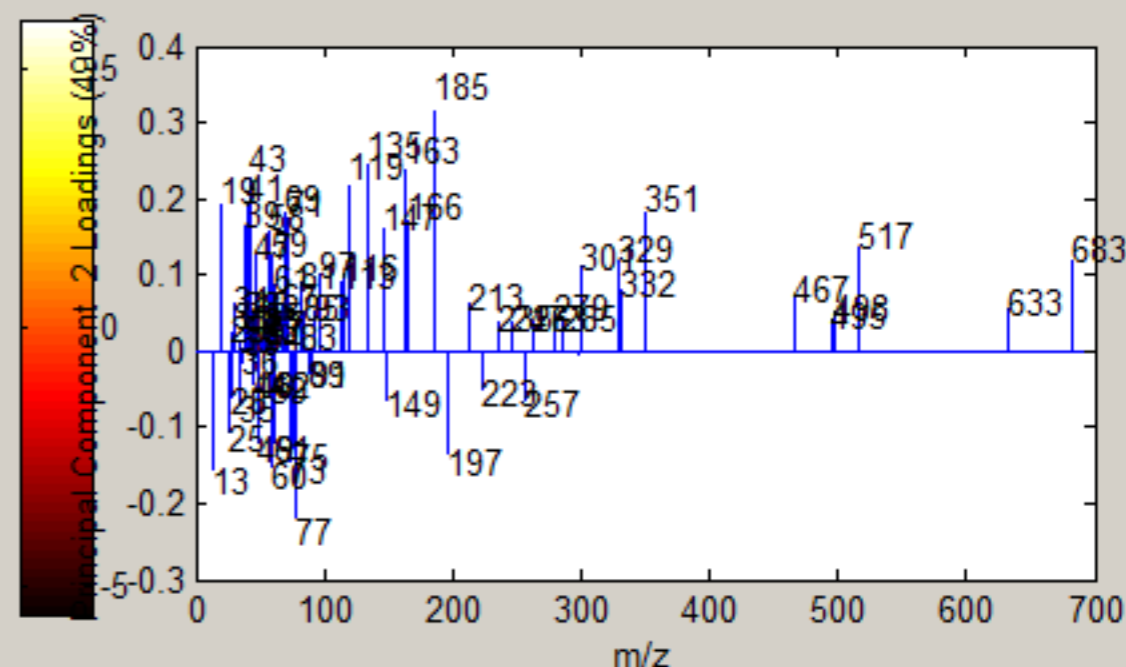
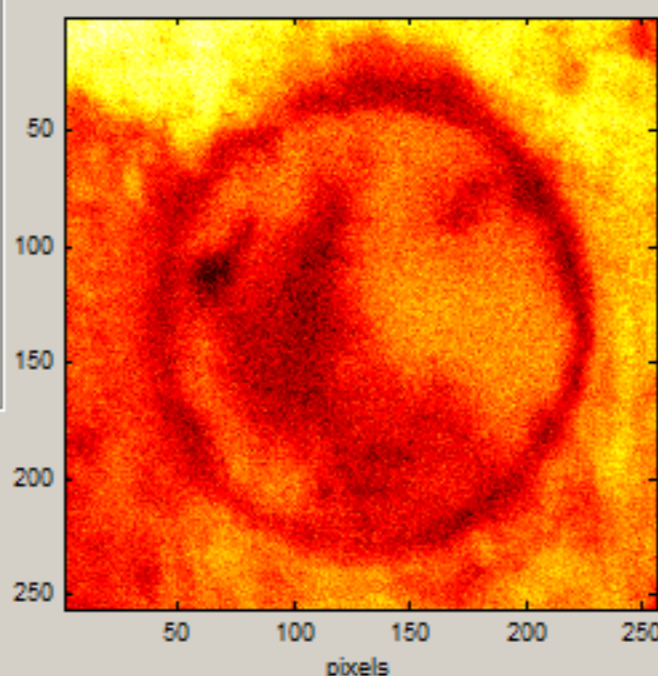
Plot Scores and Loads

Peak List

25.0083
27.9764
29.0035
30.9976
31.0197
34.9697
34.9923
36.0001
37.0082
37.9961
38.0159
39.0052
39.0251
39.9952
41.0043
42.0081

Plot Peak Area Image

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

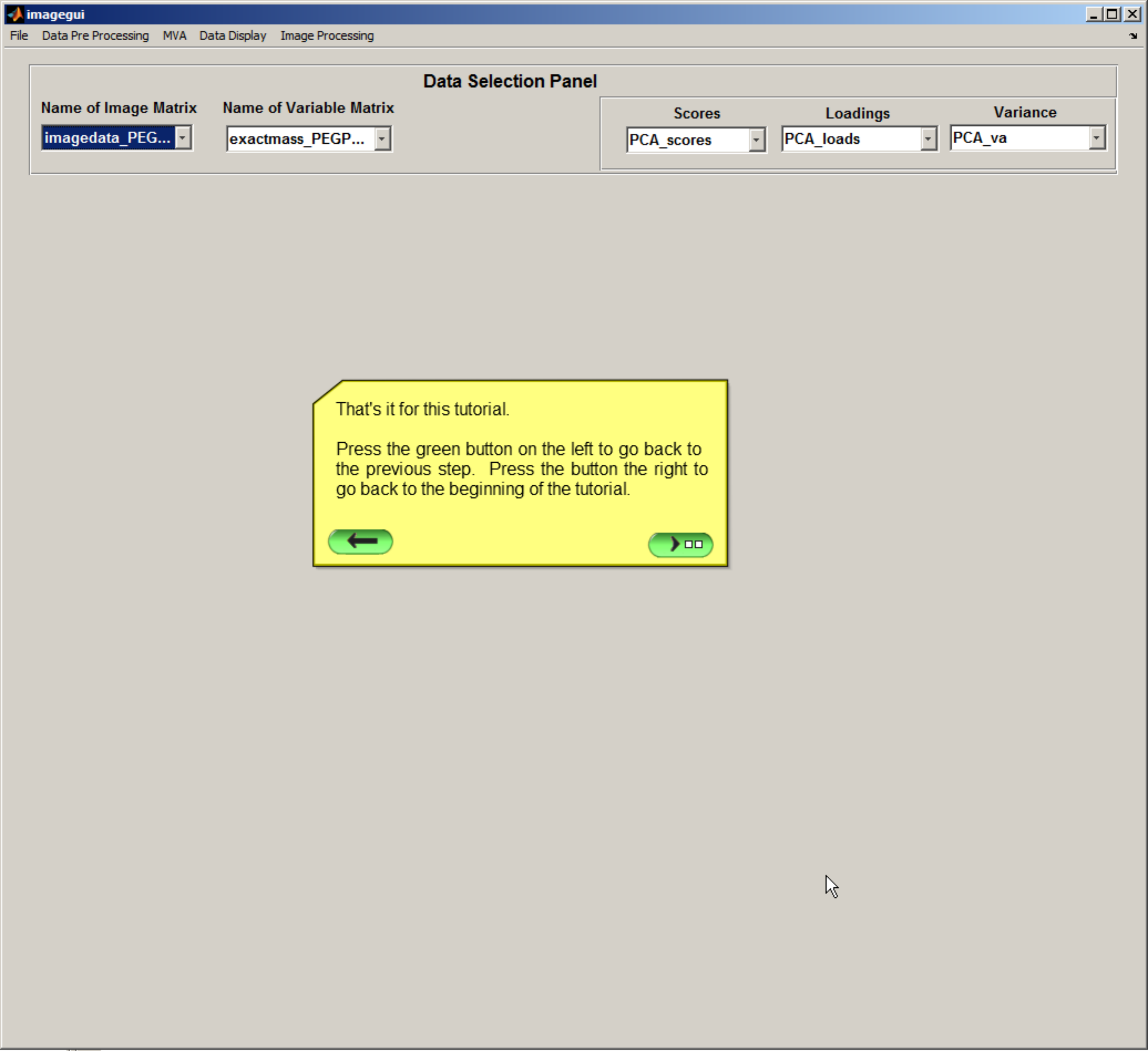


Save Figure

Make Ext

Close Panel

You can close the panel by pressing the
'Close Panel' button.



Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

imagedata_PEG...

exactmass_PEGP...

Scores

Loadings

Variance

PCA_scores

PCA_loads

PCA_va

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.

