

Data Selection Panel

Name of Image Matrix

Select Data ...

Name of Variable Matrix

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

Name of Variable Matrix

Select Data

Select Variables

This tutorial will explain some important differences between the NBToolbox in Matlab and the standalone NBToolbox that does not require Matlab.

The functions included in each version of the NBToolbox are the same, however there are some new things you need to understand in order to use the standalone version properly.

NOTE: Data files need to be in the same directory as the .exe files of the toolbox in order for the data to load properly.

Other than the issues stated in this tutorial, the tutorials for the Matlab version of the NBToolbox are valid for the standalone NBToolbox.



Current Folder		Workspace	
		Stack: Base	Select data to plot
Name		Value	
exactmass_PEGPS_07		<80x8 char>	
headerinfo_PEGPS_07		<82x4 double>	
imagedata_PEGPS_07		<65536x80 double>	
sumofselected_PEGPS_07		<65536x1 double>	
totalcounts_PEGPS_07		<65536x1 double>	

Command Window

New to MATLAB? Watch this video.

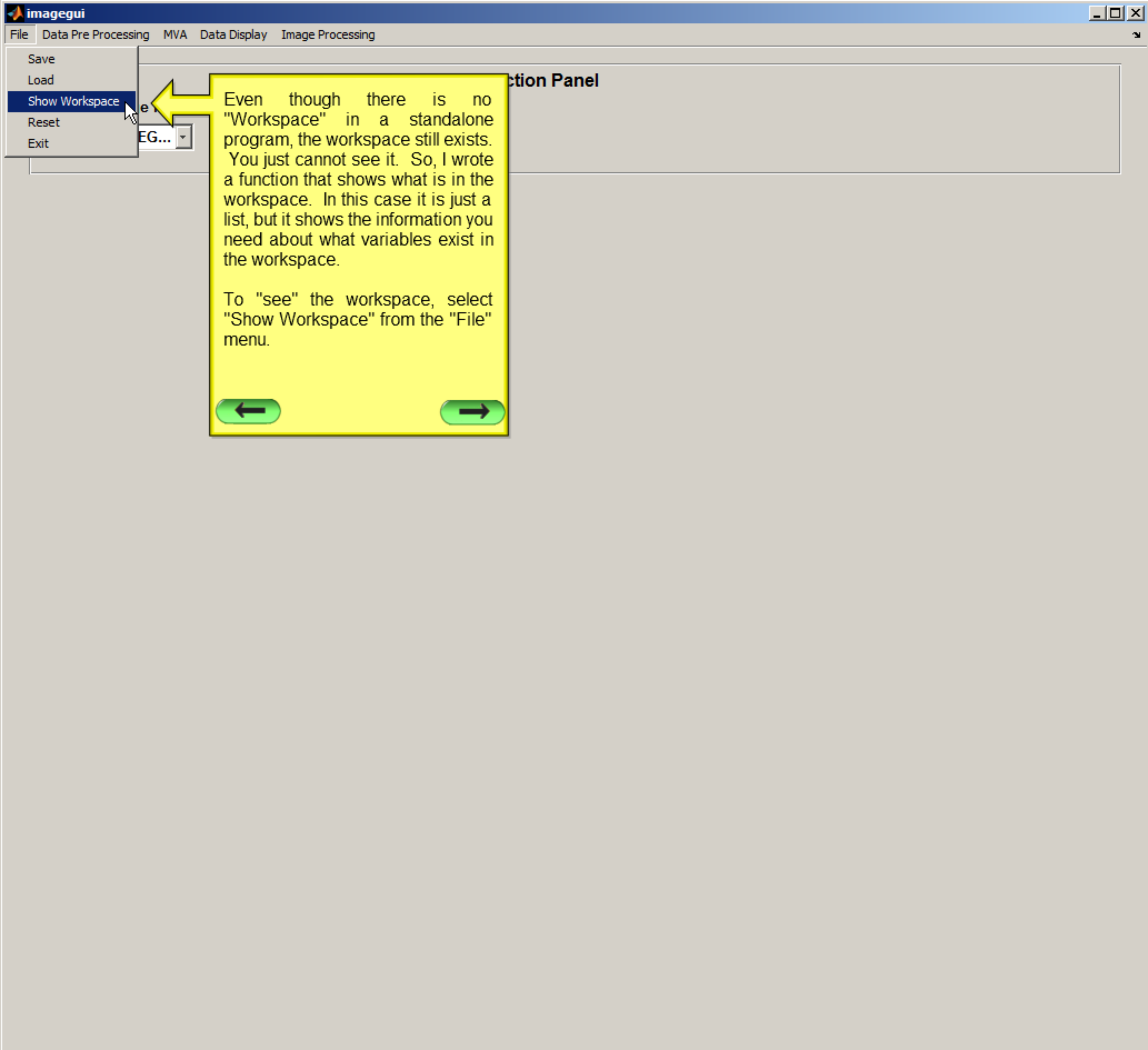
fx >>

One major difference between the standalone NBToolbox and the NBToolbox running in Matlab is that the standalone version doesn't have the Matlab command window and workspace.

This creates a few issues with how you can create new variables for labels and other places you would have to type at the Matlab command prompt.

However, I have implemented functions that get around these limitations.





Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

workspacegui

Refresh

Variable name	Size	Type

The workspacegui window will appear. Press the 'Refresh' button to show the workspace variables.



Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

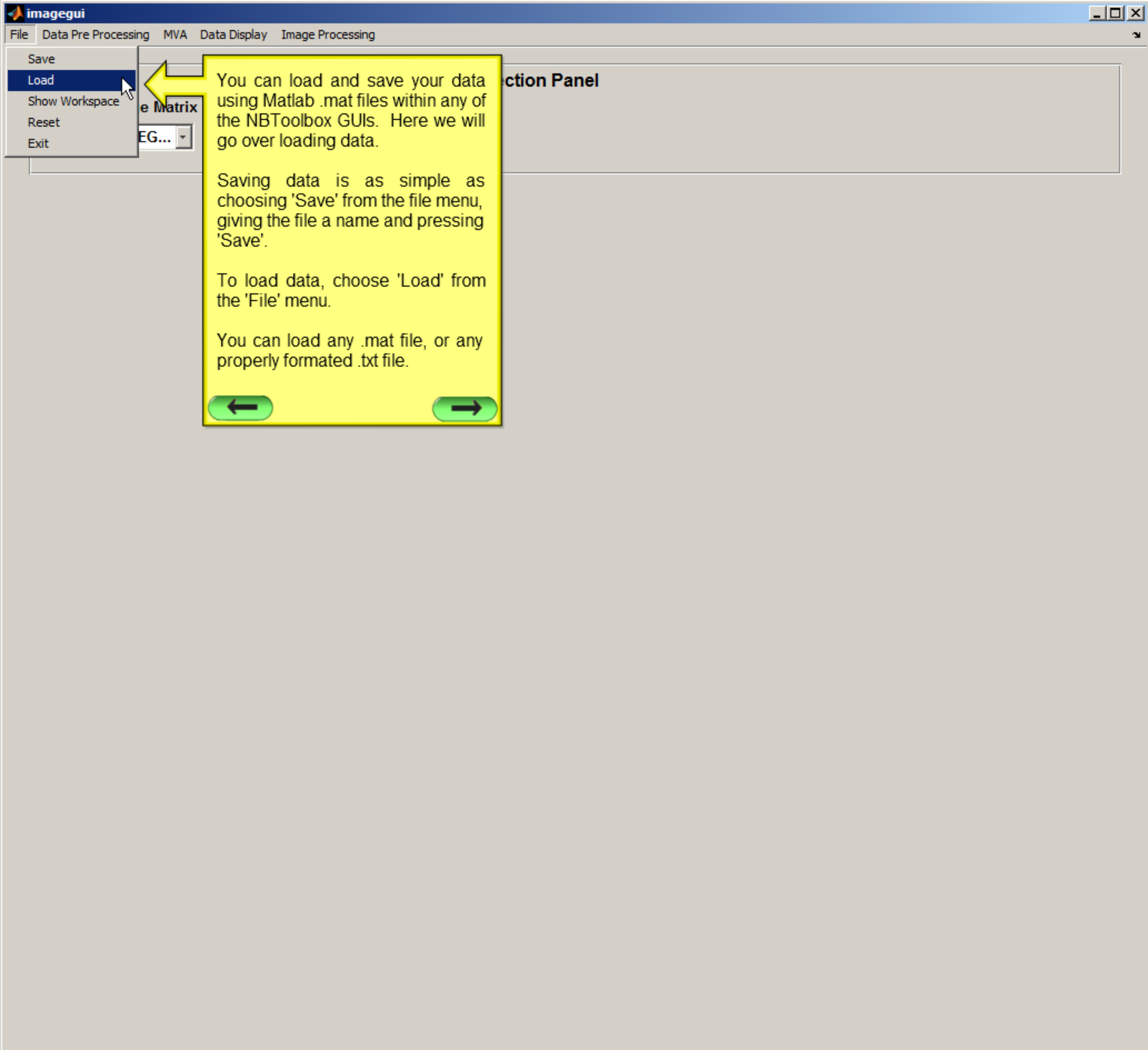
exactmass_PEGP...

workspacegui

Refresh

Variable name	Size	Type
exactmass_PEGPS_07	80x8	char
headerinfo_PEGPS_07	82x4	double
imagedata_PEGPS_07	65536x80	double
sumofselected_PEGPS...	65536x1	double
totalcounts_PEGPS_07	65536x1	double

All variables within the workspace are shown along with the typical information shown in Matlab.



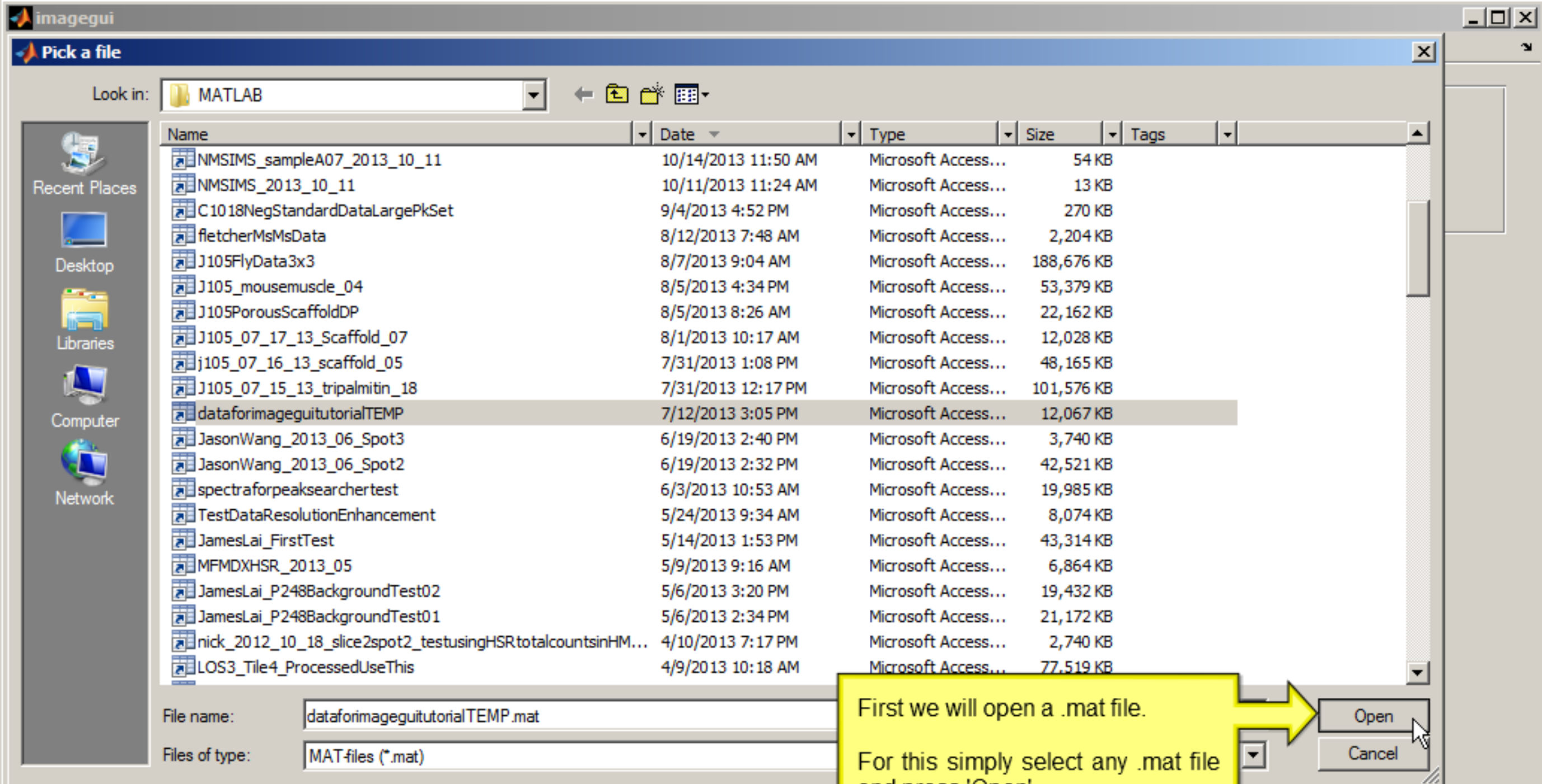
You can load and save your data using Matlab .mat files within any of the NBTtoolbox GUIs. Here we will go over loading data.

Saving data is as simple as choosing 'Save' from the file menu, giving the file a name and pressing 'Save'.

To load data, choose 'Load' from the 'File' menu.

You can load any .mat file, or any properly formatted .txt file.





Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

workspacegui

Refresh

Press the 'Refresh' button to show the workspace variables.

Variable name	Size	Type
exactmass_PEGPS_07	80x8	char
headerinfo_PEGPS_07	82x4	double
imagedata_PEGPS_07	65536x80	double
sumofselected_PEGPS...	65536x1	double
totalcounts_PEGPS_07	65536x1	double

Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

workspacegui

Refresh

Variable name	Size	Type
Lines	65536x1	double
MAF_loads	20x4	double
MAF_scores	65536x4	double
MAF_var	4x1	double
PCA_loads	20x4	double
PCA_scores	65536x4	double
PCA_var	4x1	double
PeaksIncludedIn_Lines	5x7	char
PeaksIncludedIn_squares	2x7	char
PoissonScaledMC	65536x20	double
exactmass_DAN01	20x8	char
exactmass_PEGPS_07	80x8	char
headerinfo_PEGPS_07	82x4	double
imagedata_DAN01	65536x20	double
imagedata_PEGPS_07	65536x80	double
squares	65536x1	double
sumofselected_DAN01	65536x1	double
sumofselected_PEGPS_07	65536x1	double
totalcounts_DAN01	65536x1	double
totalcounts_PEGPS_07	65536x1	double

You can see that the variables from the opened file have been added to the workspace.

You can load them into the GUI you are using with the 'Import From Workspace' functions of the Imagegui or Spectragui.



Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

Select Scores

Loadings

PCA_loads

Variance

PCA_var

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: PCA_loads
Variables: exactmass_PEGPS_07
% Variance: PCA_var

PC# to plot

1

Plot Options:

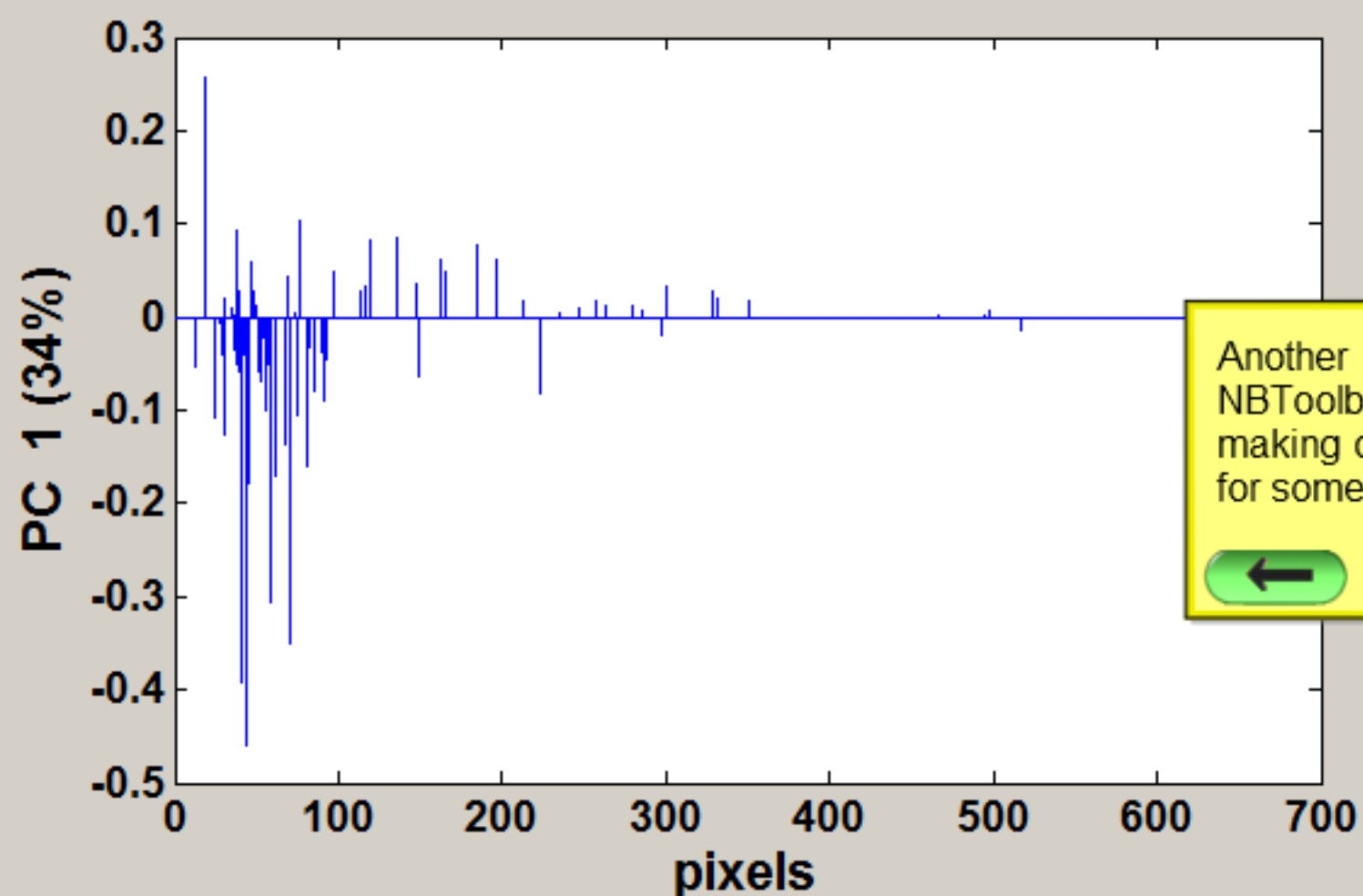
Traditional

Plot Loads

Save Figure

Make Ext

Close Panel



Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Image size (microns):

Create Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

Label Custom

Another issue with the standalone NBToolbox is how to deal with making custom labels or peak lists for some functions.



Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

labelstest.txt - Notepad

File Edit Format View Help

this
is
a
test

Scores

Select Scores

Loadings

PCA_loads

Variance

PCA_var

Load Select

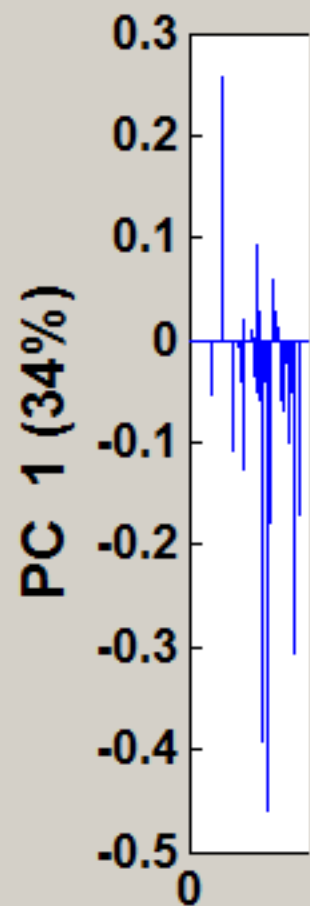
Load Select

PC# to plot

1

Plot Options:

Traditional



For this you will need to use a text editor and create a .txt file that contains the labels or peak lists you want to import into the NBToolbox.

Remember that each label or peak mass must be on a separate row and that all text must contain the same number of characters. This means that you must use spaces to adjust the number of characters if some text is shorter than the rest.

In this example I used spaces to make sure that each line of text is the same length.

el Loadings

above
value.

Label Threshold

microns):

Create Raw Data Plot For Labeled Peaks

Use custom labels
for selected peaks.

Custom Labels
to use

Choose Peaks

Label Custom

Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

labelstest.txt - Notepad

File Edit Format View Help

this
is
a
test

Scores

Loadings

Variance

loads

PCA_var

Save this as a .txt file. The name you give to the file will become the name of the variable in the workspace that contains the labels/peaks/etc.



Load Select

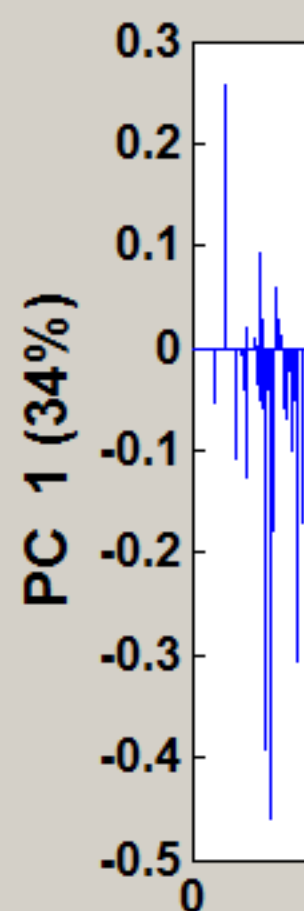
Load Select

PC# to plot

1

Plot Options:

Traditional



Label Loadings

Label all peaks above
a threshold value.

Label Peaks
Above

Label Threshold

Image size (microns):

Create Raw Data Plot For Labeled Peaks

Use custom labels
for selected peaks.

Custom Labels
to use

Choose Peaks

Label Custom

imagegui File Data Pre Processing MVA Data Display Image Processing

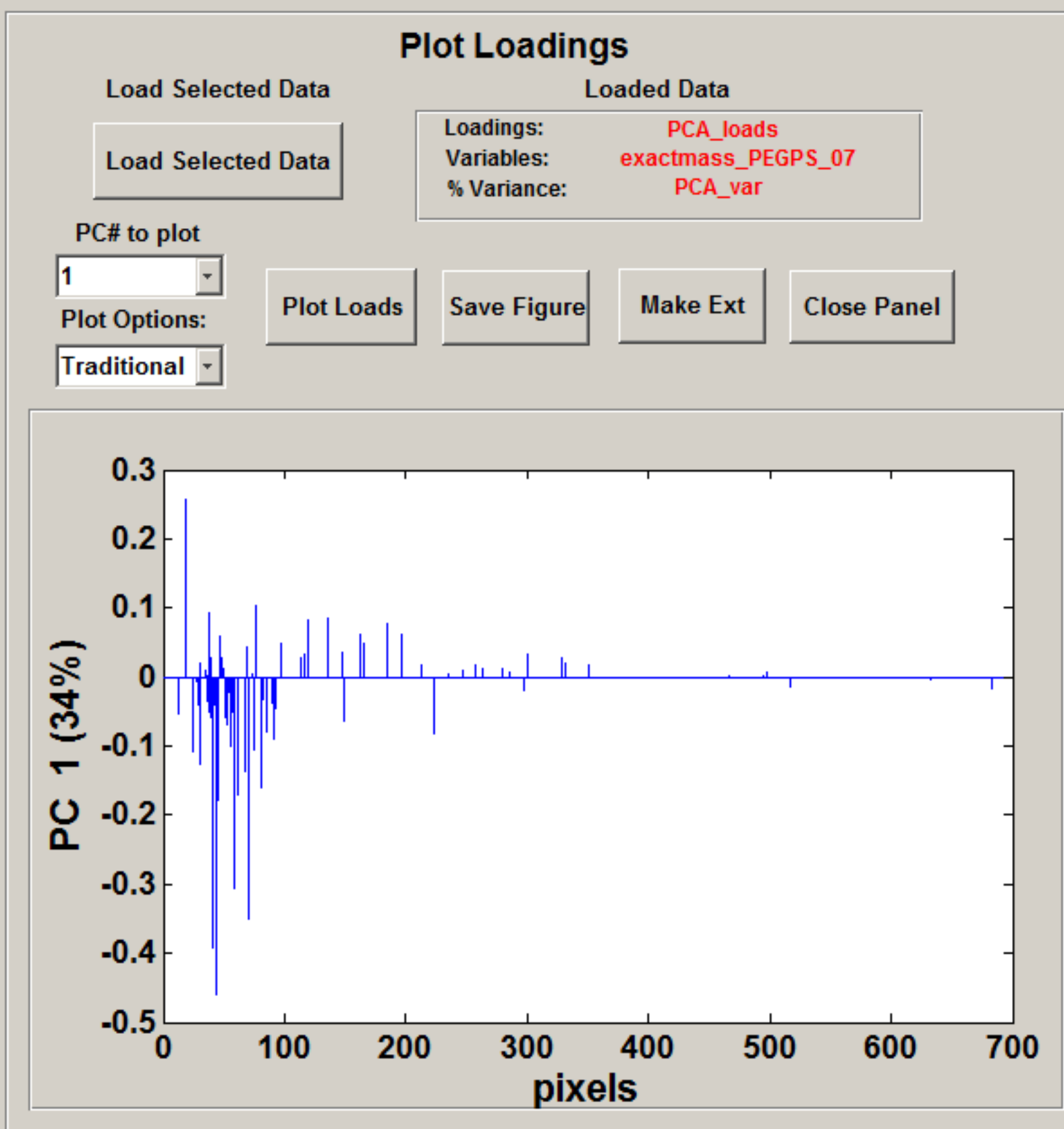
Save
Load
Show Workspace
Reset
Exit

File Matrix
EG...

To bring the data into the GUI, select 'Load' from the 'File' menu.

Section Panel

Scores Loadings Variance
Select Scores PCA_loads PCA_var



Label Loadings

Label all peaks above a threshold value.

Label Peaks Above
Label Threshold

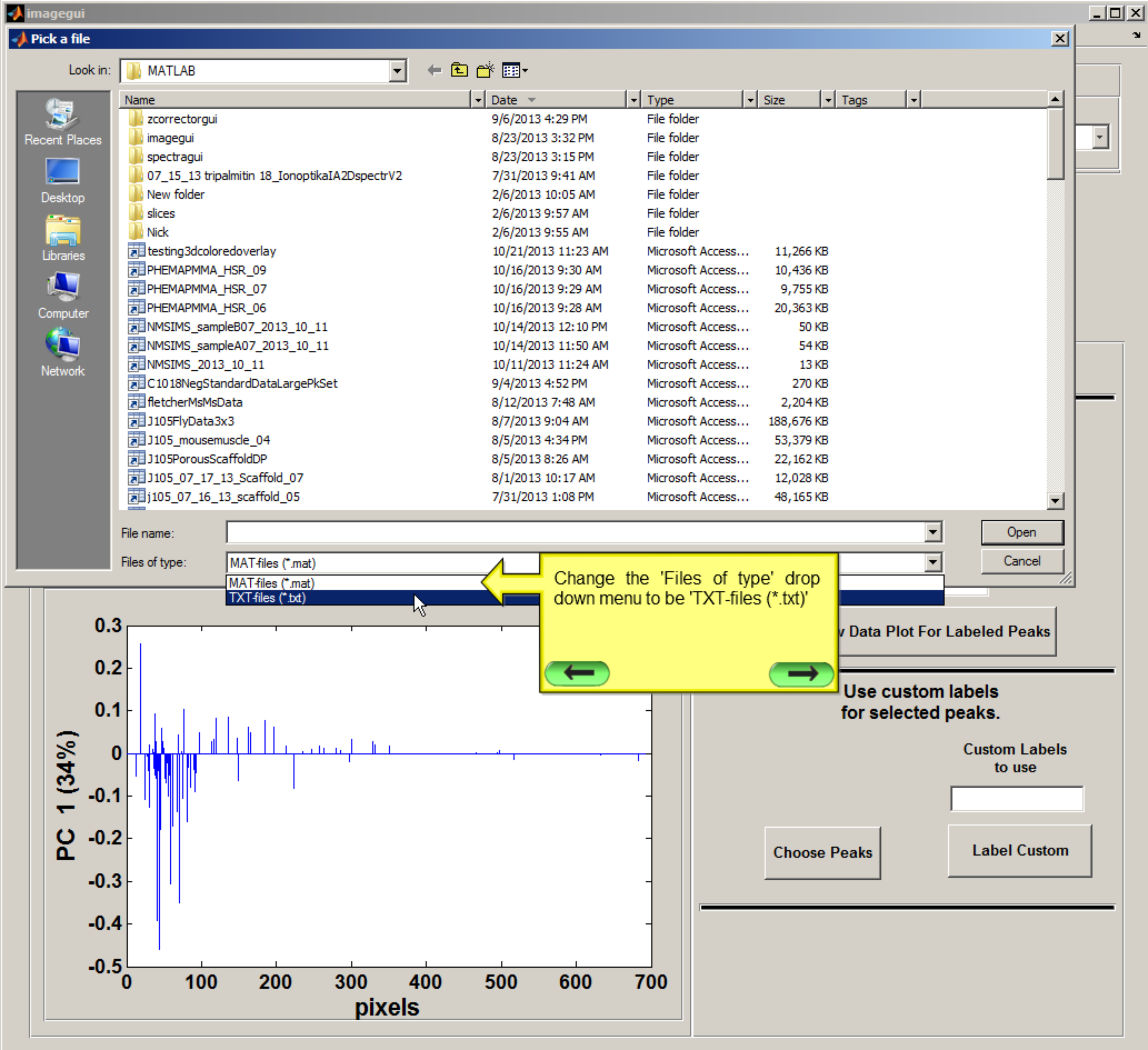
Image size (microns):

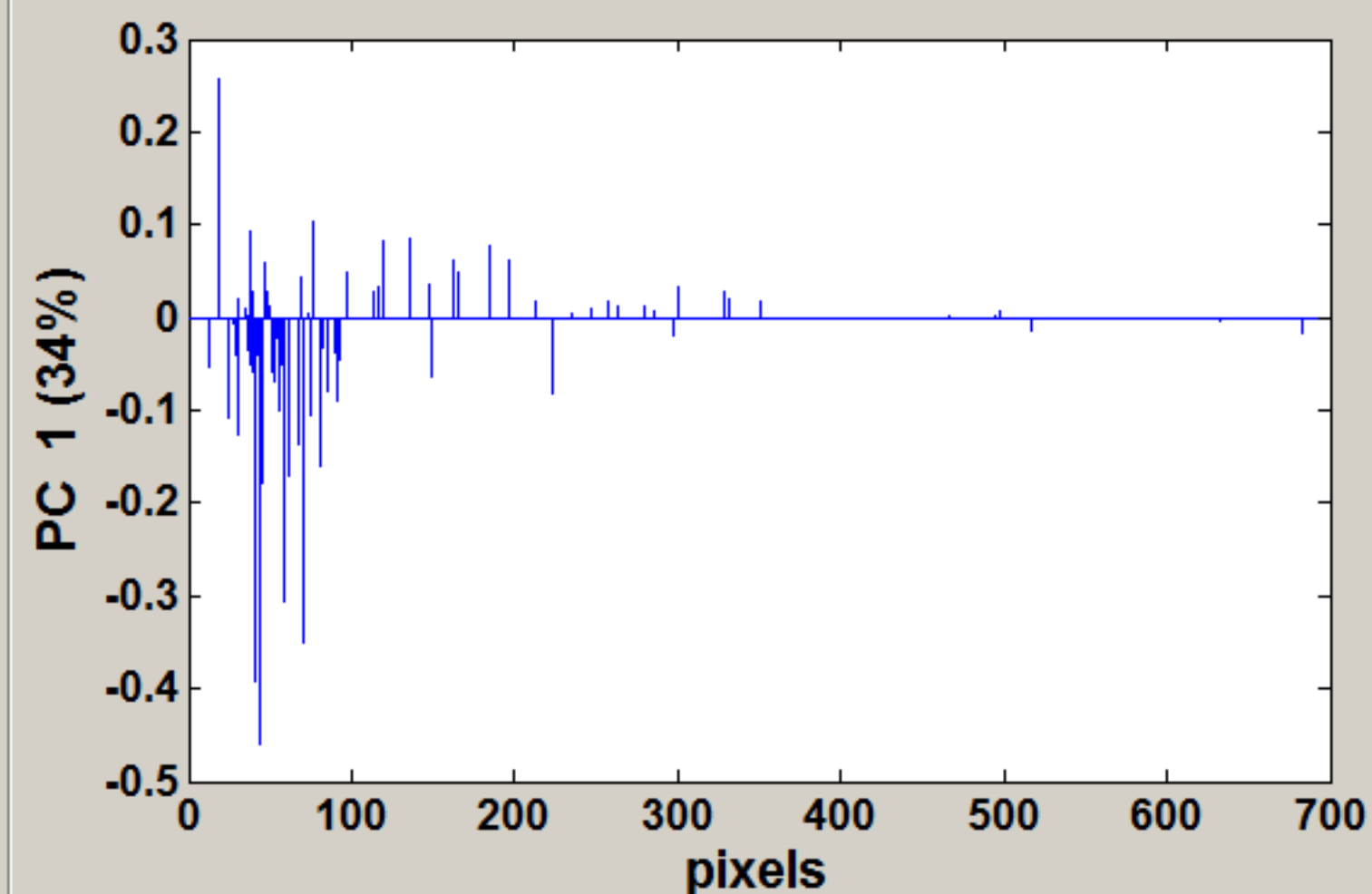
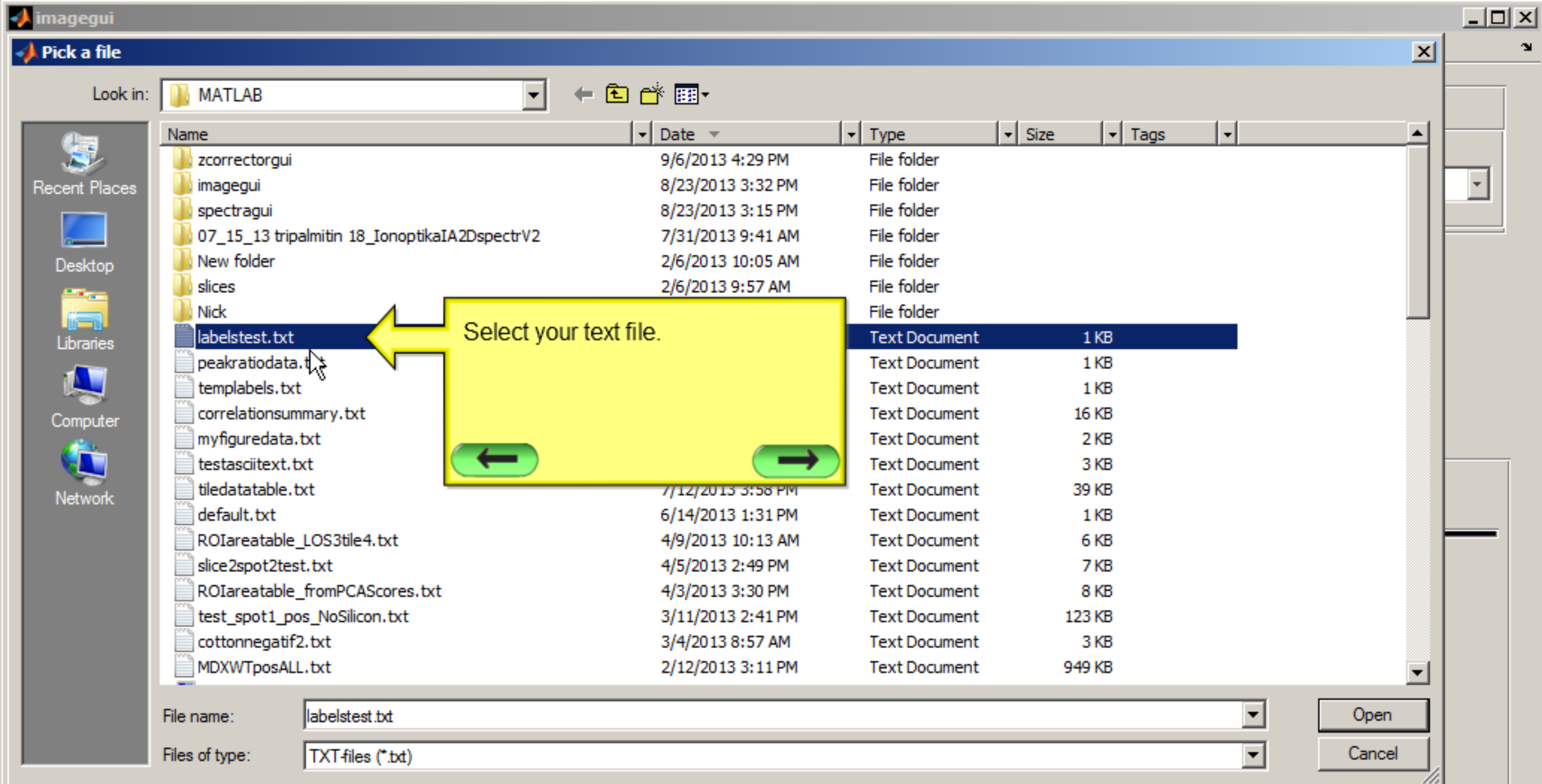
Create Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

Choose Peaks Label Custom





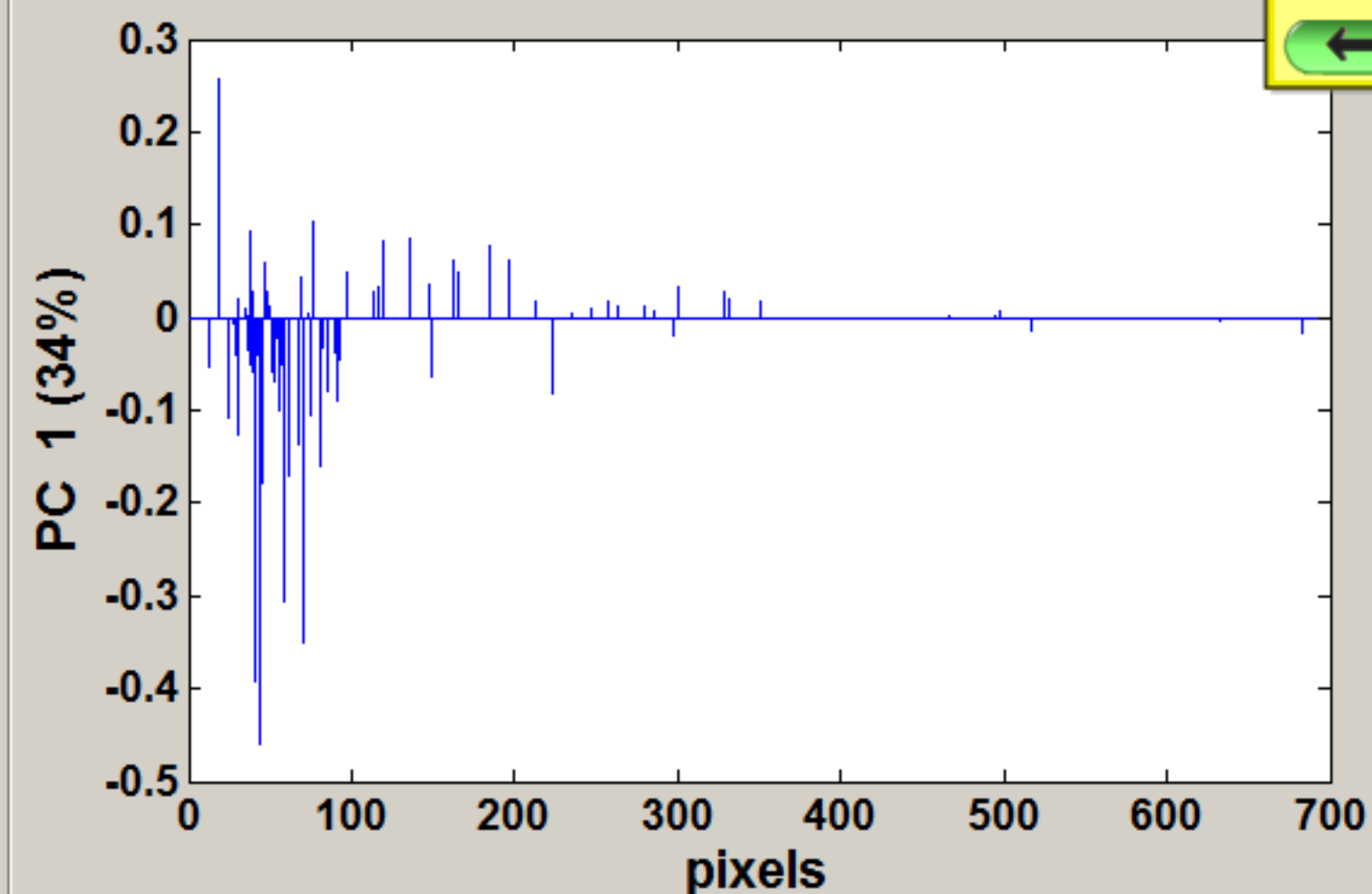
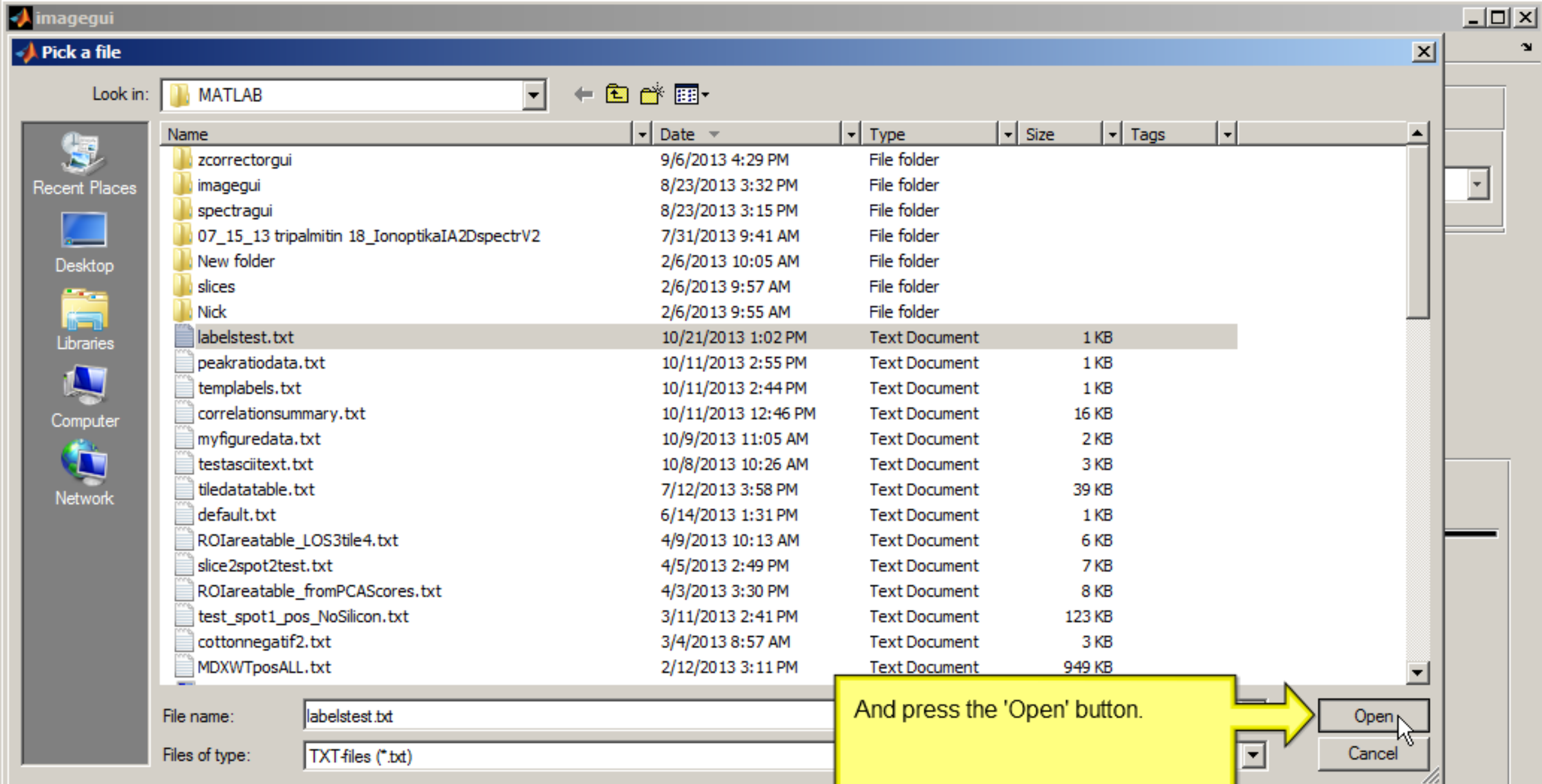
Create Raw Data Plot For Labeled Peaks

Use custom labels
for selected peaks.

Custom Labels
to use

Choose Peaks

Label Custom



For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

Choose Peaks

Label Custom

Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

Select Scores

Loadings

PCA_loads

Variance

PCA_var

workspacegui

Press the 'Refresh' button to refresh the variable list.

Refresh

Variable name	Size	Type
	65536x1	double
ls	20x4	double
MAF_scores	65536x4	double
MAF_var	4x1	double
PCA_loads	20x4	double
PCA_scores	65536x4	double
PCA_var	4x1	double
PeaksIncludedIn_Lines	5x7	char
PeaksIncludedIn_squares	2x7	char
PoissonScaledMC	65536x20	double
exactmass_DAN01	20x8	char
exactmass_PEGPS_07	80x8	char
headerinfo_PEGPS_07	82x4	double
imagedata_DAN01	65536x20	double
imagedata_PEGPS_07	65536x80	double
squares	65536x1	double
sumofselected_DAN01	65536x1	double
sumofselected_PEGPS_07	65536x1	double
totalcounts_DAN01	65536x1	double
totalcounts_PEGPS_07	65536x1	double

Label Loadings

Label all peaks above threshold value.

Label Peaks Above

Label Threshold

Image size (microns):

Create Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

Choose Peaks

Label Custom

Load Selected Data

Load Selected Data

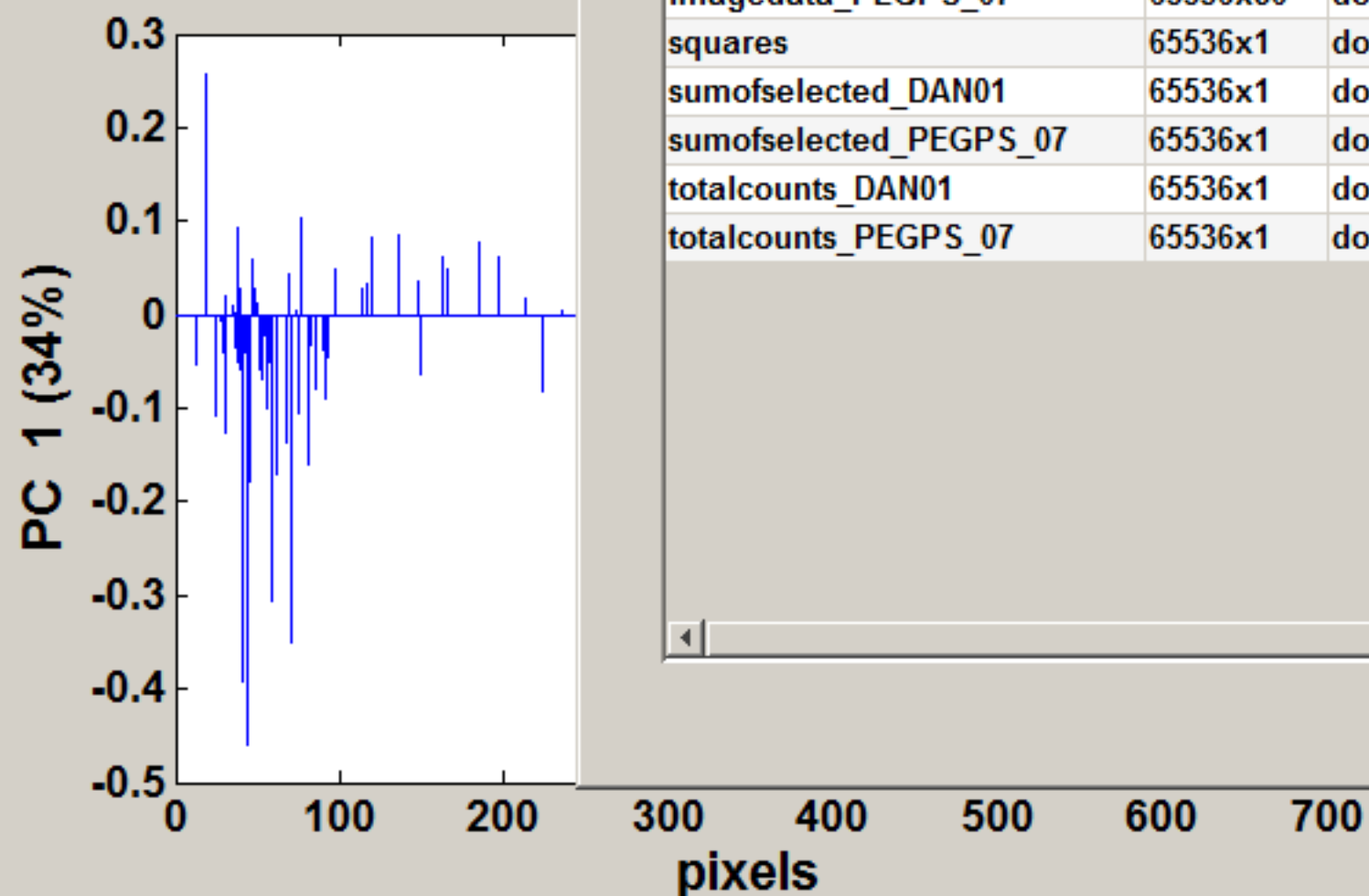
PC# to plot

1

Plot Options:

Traditional

Plot Loads



Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

Select Scores

Loadings

PCA_loads

Variance

PCA_var

workspacegui

Refresh

Variable name	Size	Type
Lines	65536x1	double
MAF_loads	20x4	double
MAF_scores	65536x4	double
MAF_var	4x1	double
PCA_loads	80x4	double
PCA_scores	65536x4	double
PCA_var	4x1	double
PeaksIncludedIn_Lines	5x7	char
PeaksIncludedIn_squares	2x7	char
PoissonScaledMC	65536x20	double
SquareRootMC	65536x80	double
exactmass_DAN01	20x8	char
exactmass_PEGPS_07	80x8	char
headerinfo_PEGPS_07	82x4	double
imagedata_DAN01	65536x20	double
imagedata_PEGPS_07	65536x80	double
labelstest	4x4	char
squares	65536x1	double
sumofselected_DAN01	65536x1	double
sumofselected_PEGPS_07	65536x1	double
totalcounts_DAN01	65536x1	double
totalcounts_PEGPS_07	65536x1	double

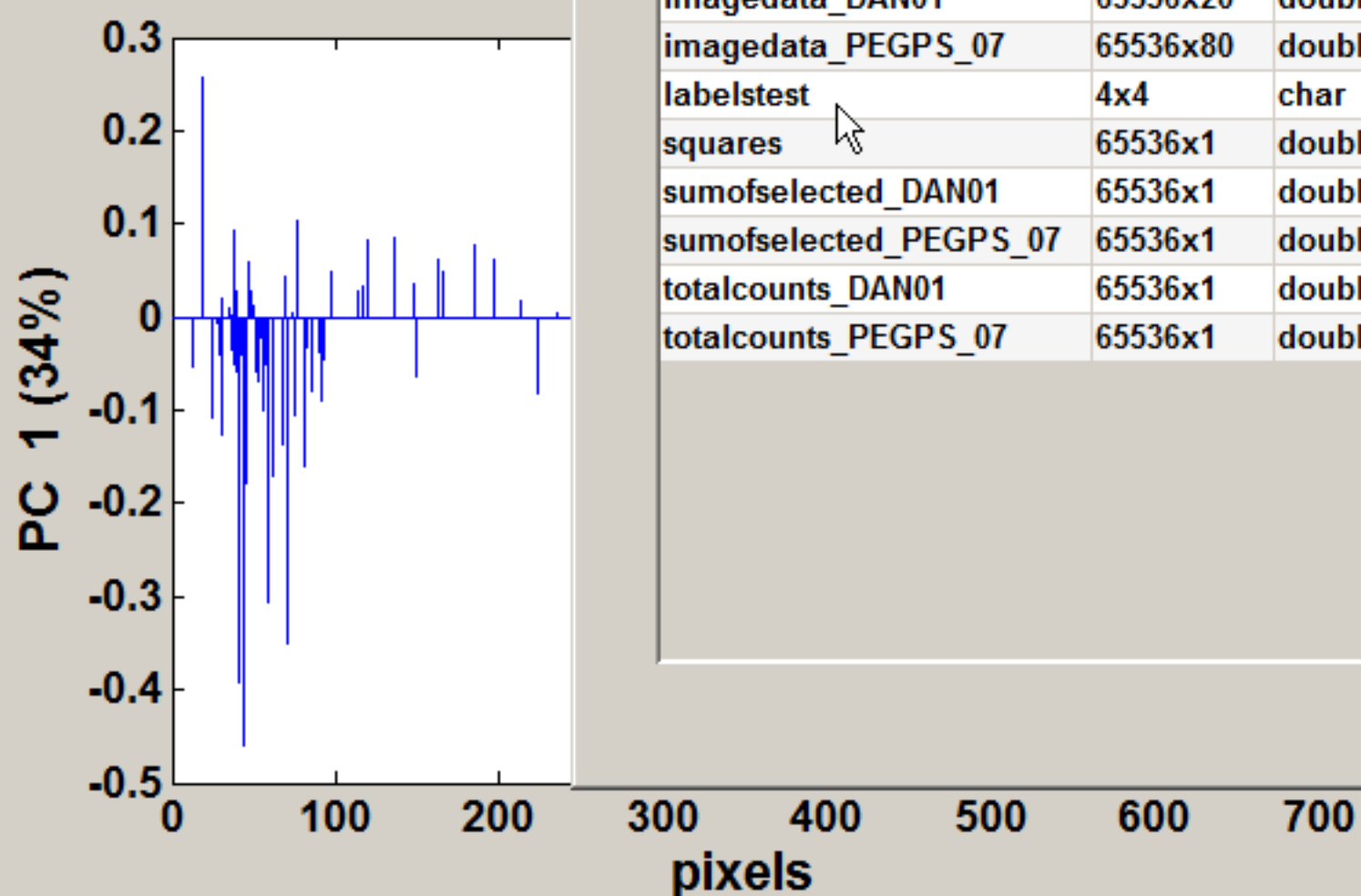
Label Loadings

Label all peaks above threshold value.

Label Peaks Above

Label Threshold

Image size (microns):



And you can see the file had been loaded and saved as a new variable using the name of the file.



Choose Peaks

Label Custom

Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

Select Scores

Loadings

PCA_loads

Variance

PCA_var

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: PCA_loads
Variables: exactmass_PEGPS_07
% Variance: PCA_var

PC# to plot

1

Plot Options:

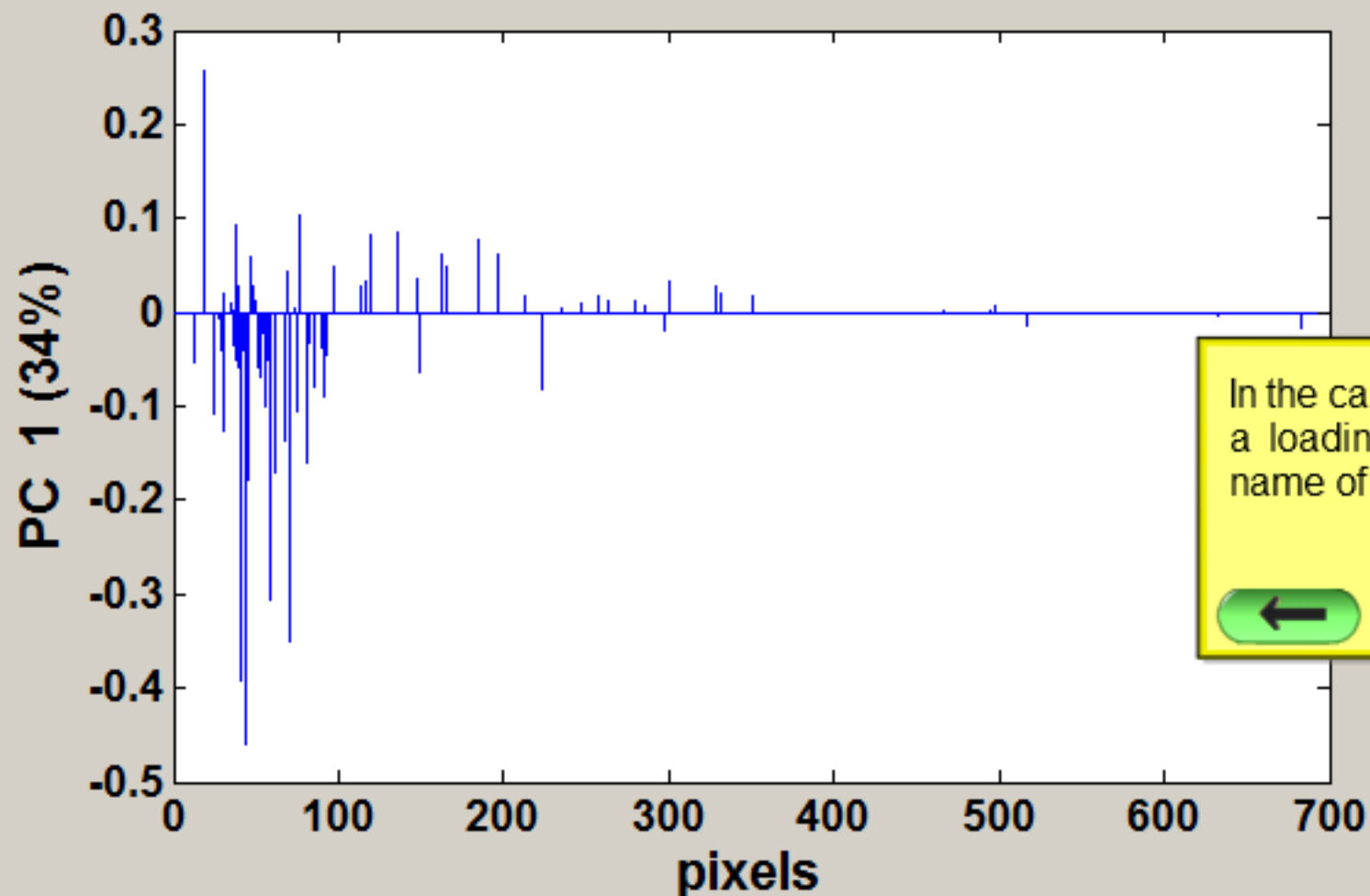
Traditional

Plot Loads

Save Figure

Make Ext

Close Panel



Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Image size (microns):

Create Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

labelstest

Name of variable

Label Custom

In the case of the custom labels for a loadings plot, we can enter the name of the variable here.

Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

Select Scores

Loadings

PCA_loads

Variance

PCA_var

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: PCA_loads
Variables: exactmass_PEGPS_07
% Variance: PCA_var

PC# to plot

1

Plot Options:

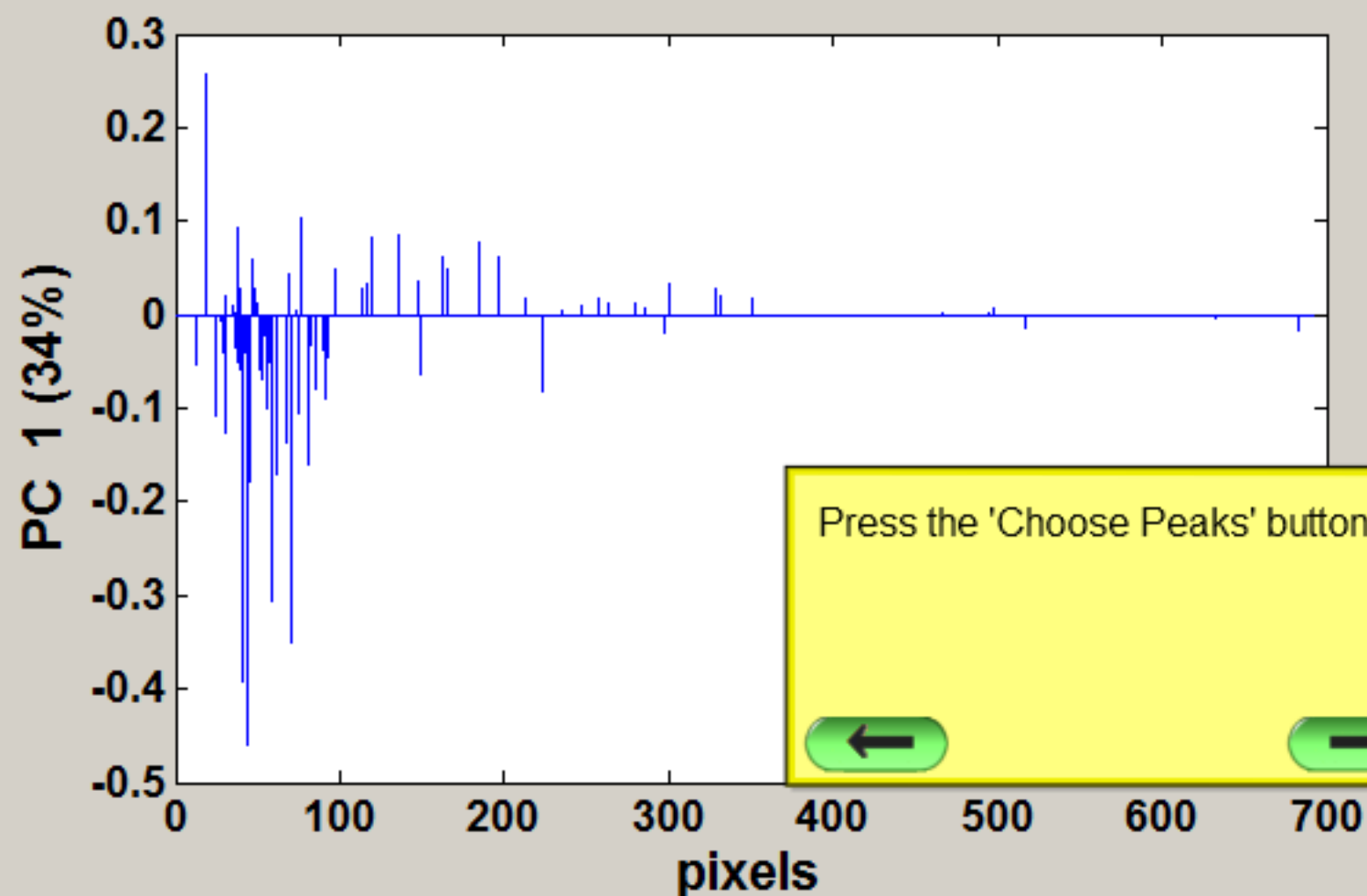
Traditional

Plot Loads

Save Figure

Make Ext

Close Panel



Press the 'Choose Peaks' button.

Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Image size (microns):

Create Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

labelstest

Label Custom

Choose Peaks

Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

Select Scores

Loadings

PCA_loads

Variance

PCA_var

Plot Loadings

Load Selected Data

Load Selected Data

PC# to plot

1

Plot Options:

Traditional

Loaded Data

Loadings: PCA_loads
Variables: exactmass_PEGPS_07
% Variance: PCA_var

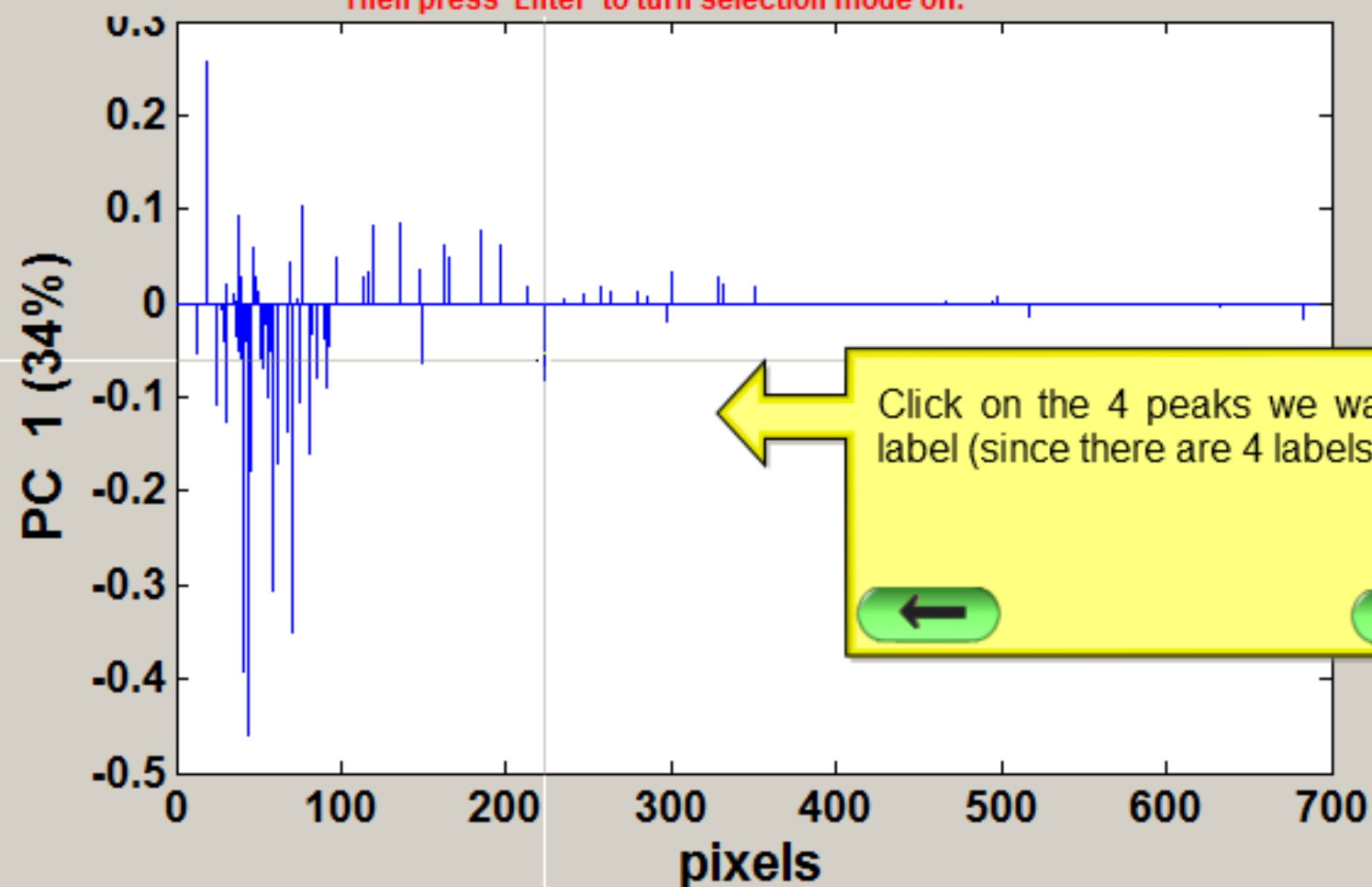
Plot Loads

Save Figure

Make Ext

Close Panel

Click on a peak where you want the label to appear to add it to the selection.
Then press 'Enter' to turn selection mode off.



Click on the 4 peaks we want to label (since there are 4 labels).

Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Image size (microns):

Create Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

labelstest

Choose Peaks

Label Custom

Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

Select Scores

Loadings

PCA_loads

Variance

PCA_var

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: PCA_loads
Variables: exactmass_PEGPS_07
% Variance: PCA_var

PC# to plot

1

Plot Options:

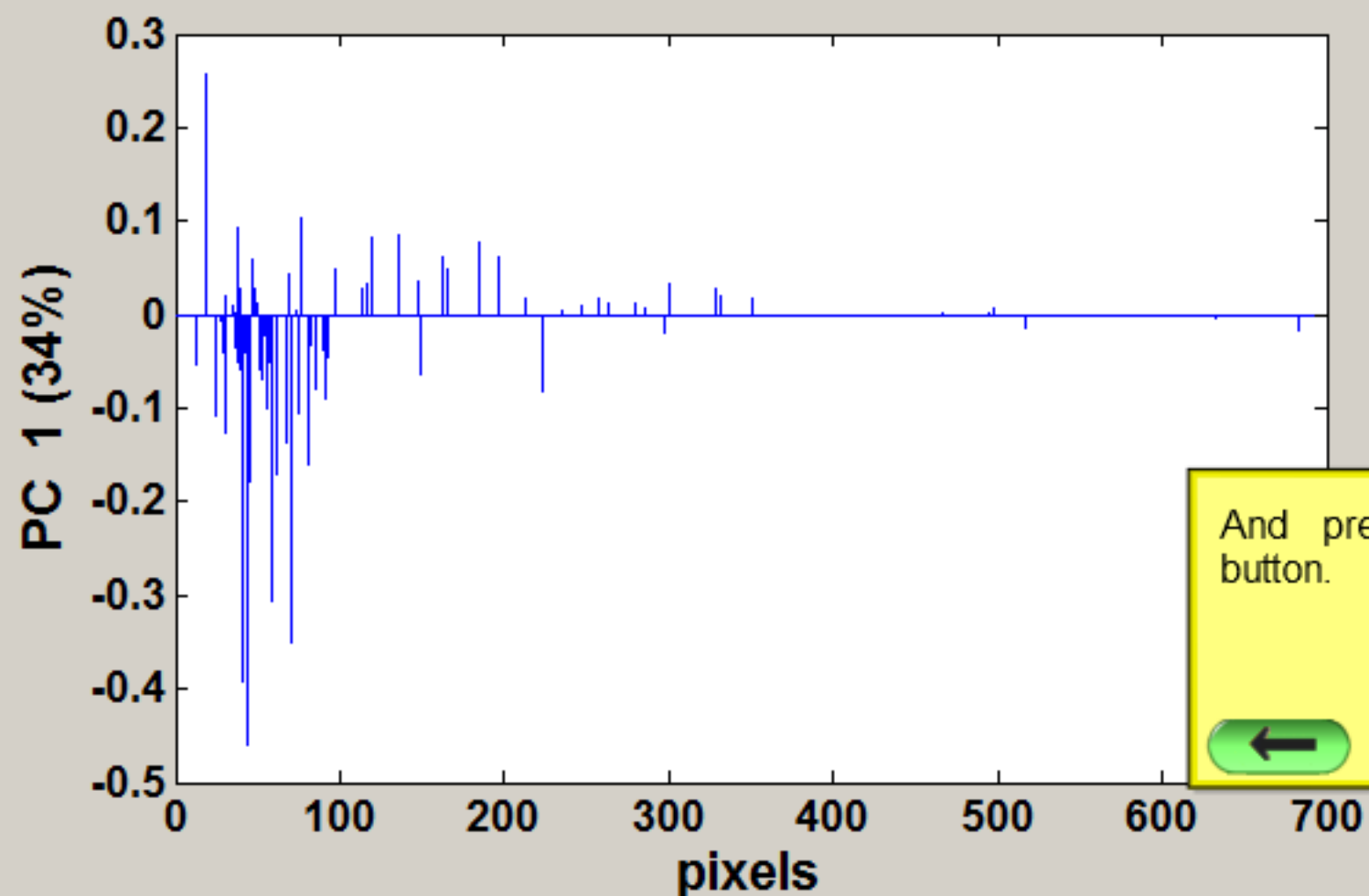
Traditional

Plot Loads

Save Figure

Make Ext

Close Panel



Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Image size (microns):

Create Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

labelstest

Label Custom

And press the 'Label Custom' button.

Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

Select Scores

Loadings

PCA_loads

Variance

PCA_var

Plot Loadings

Load Selected Data

Load Selected Data

Loaded Data

Loadings: PCA_loads
Variables: exactmass_PEGPS_07
% Variance: PCA_var

PC# to plot

1

Plot Options:

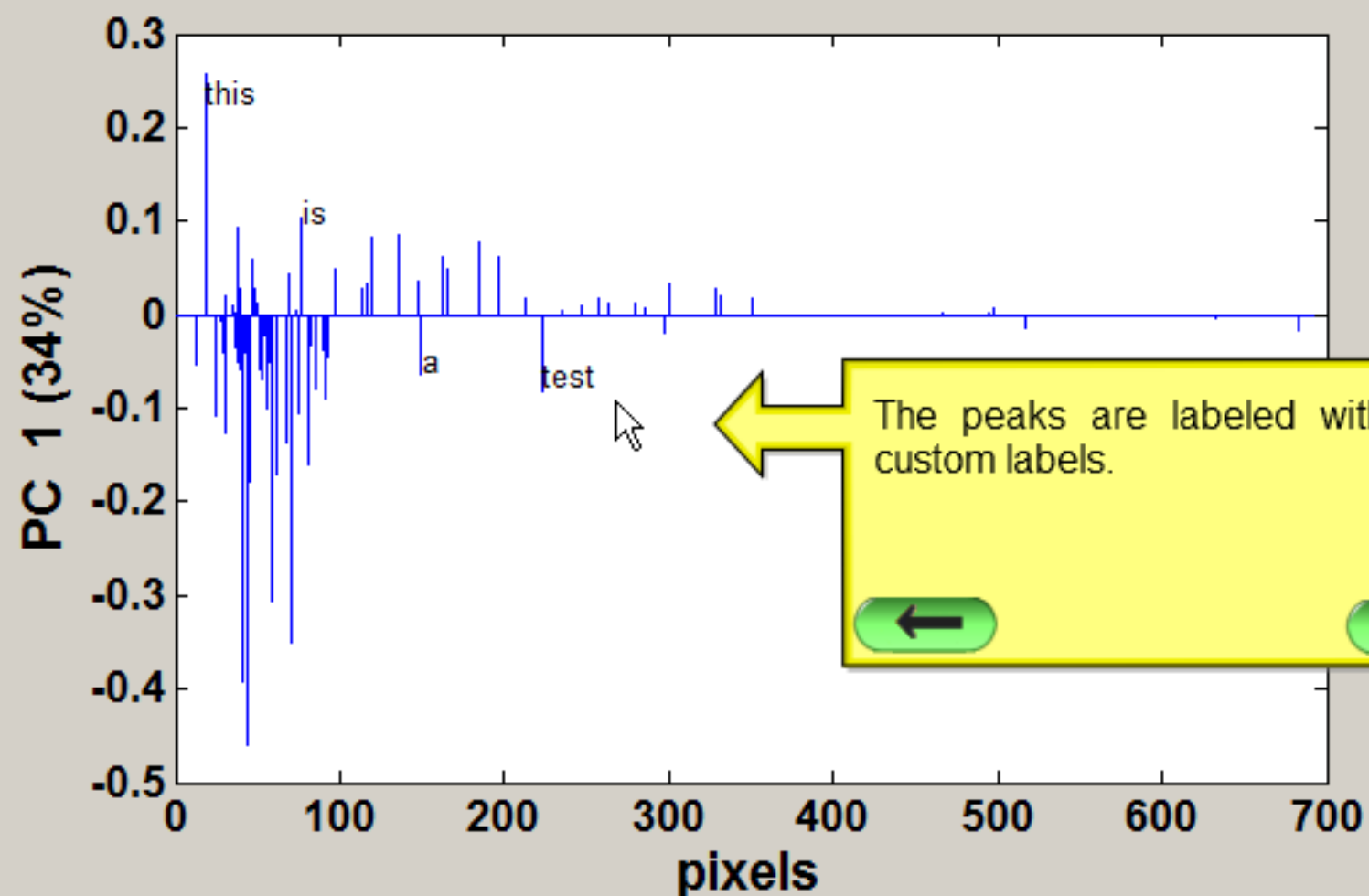
Traditional

Plot Loads

Save Figure

Make Ext

Close Panel



Label Loadings

Label all peaks above a threshold value.

Label Peaks Above

Label Threshold

Image size (microns):

Create Raw Data Plot For Labeled Peaks

Use custom labels for selected peaks.

Custom Labels to use

labelstest

Choose Peaks

Label Custom

Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

Select Scores

Loadings

PCA_loads

Variance

PCA_var

Though this tutorial used the imagegui for demonstration purposes, the functions described work the same within the spectragui.



Data Selection Panel

Name of Image Matrix

imagedata_PEG...

Name of Variable Matrix

exactmass_PEGP...

Scores

Select Scores

Loadings

PCA_loads

Variance

PCA_var

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.

Please see the other imagegui and spectragui tutorials for detailed information on how to use the functions within the NBToolbox.

