

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_e2n...

Name of Variable Matrix

exactmass_e2n_1 ...

This tutorial covers how to run MCR using the Imagegui.

NOTE: I did not write the code for the implementation of MCR used in the Imagegui. I am using the MCR-ALS toolbox developed by Roma Tauler and Anna de Juan from the University of Barcelona.

The MCR-ALS toolbox can be downloaded here:

<http://mcrals.info>

This must be installed before you can use the MCR panel in the Imagegui.

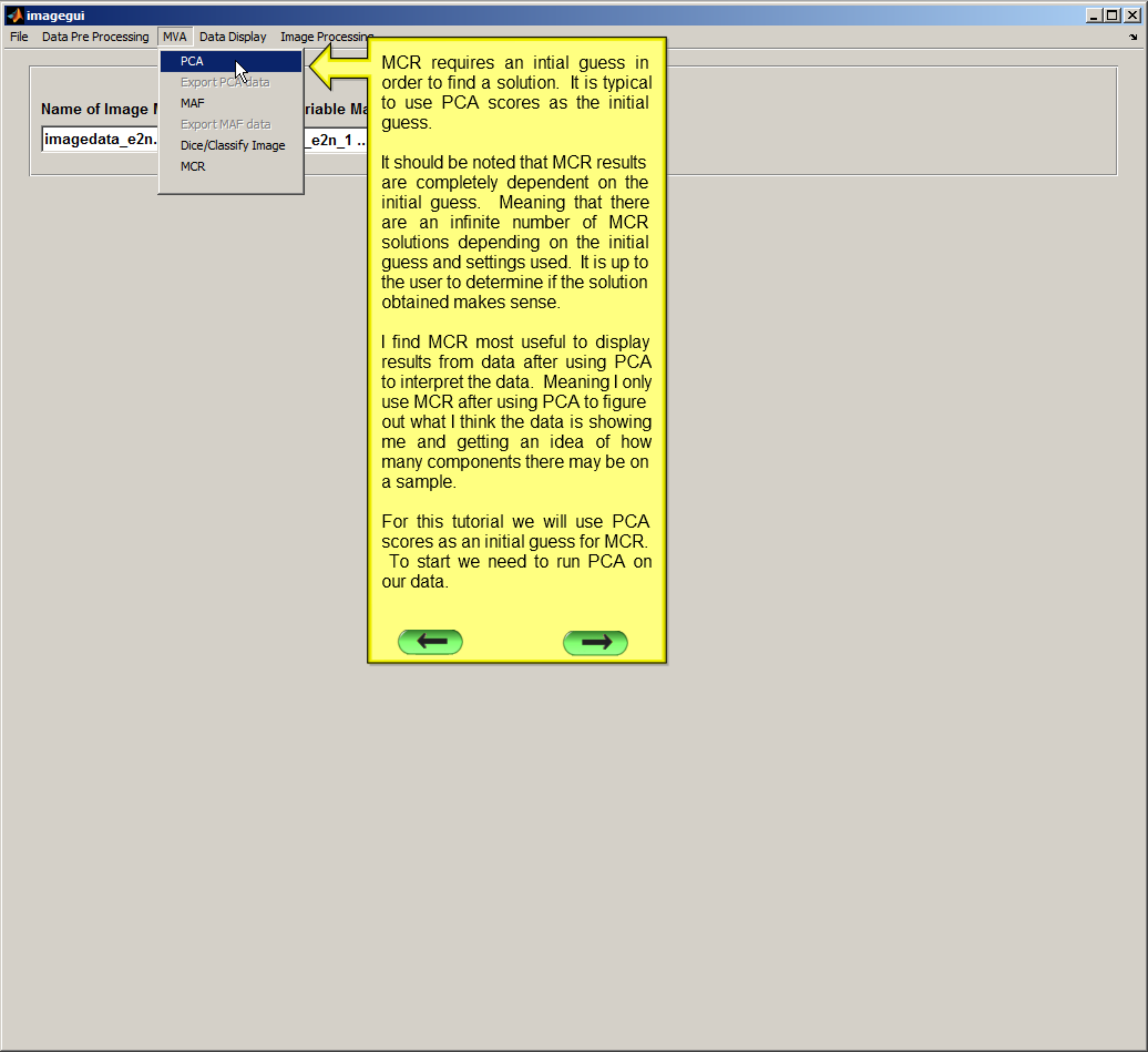
I do not use all of the options available in the MCR-ALS toolbox. If you need access to those, you will need to use the MCR-ALS toolbox directly.

My implementation of the MCR-ALS toolbox uses the following defaults:

- Non negativity for components and spectra
- Fast non linear least squares (fnnls)
- No closure

See the MCR-ALS website for more information on those settings.





MCR requires an initial guess in order to find a solution. It is typical to use PCA scores as the initial guess.

It should be noted that MCR results are completely dependent on the initial guess. Meaning that there are an infinite number of MCR solutions depending on the initial guess and settings used. It is up to the user to determine if the solution obtained makes sense.

I find MCR most useful to display results from data after using PCA to interpret the data. Meaning I only use MCR after using PCA to figure out what I think the data is showing me and getting an idea of how many components there may be on a sample.

For this tutorial we will use PCA scores as an initial guess for MCR. To start we need to run PCA on our data.



Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

imagedata_e2n...

exactmass e2n 1 ...

Load Selected Data

Image:

None

Variables

None

Data Preprocessing

Choose an option below

Run PCA

PCA Summary

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

Name for scores matrix

Name for loadings matrix

Name for Variance matrix

of PCs to keep in model

Save PCA Data

Close Panel

A detailed tutorial on running PCA can be found in tutorial 06. Here we will just cover the basics required in order to use MCR.

Select the data you want to use from the menus above and press the 'Load Selected Data' button.

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

imagedata_e2n...

exactmass_e2n_1 ...

Load Selected Data

Image: **imagedata_e2n_1**

Variables **exactmass_e2n_1**

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

Name for scores matrix

Name for loadings matrix

Name for Variance matrix

of PCs to keep in model

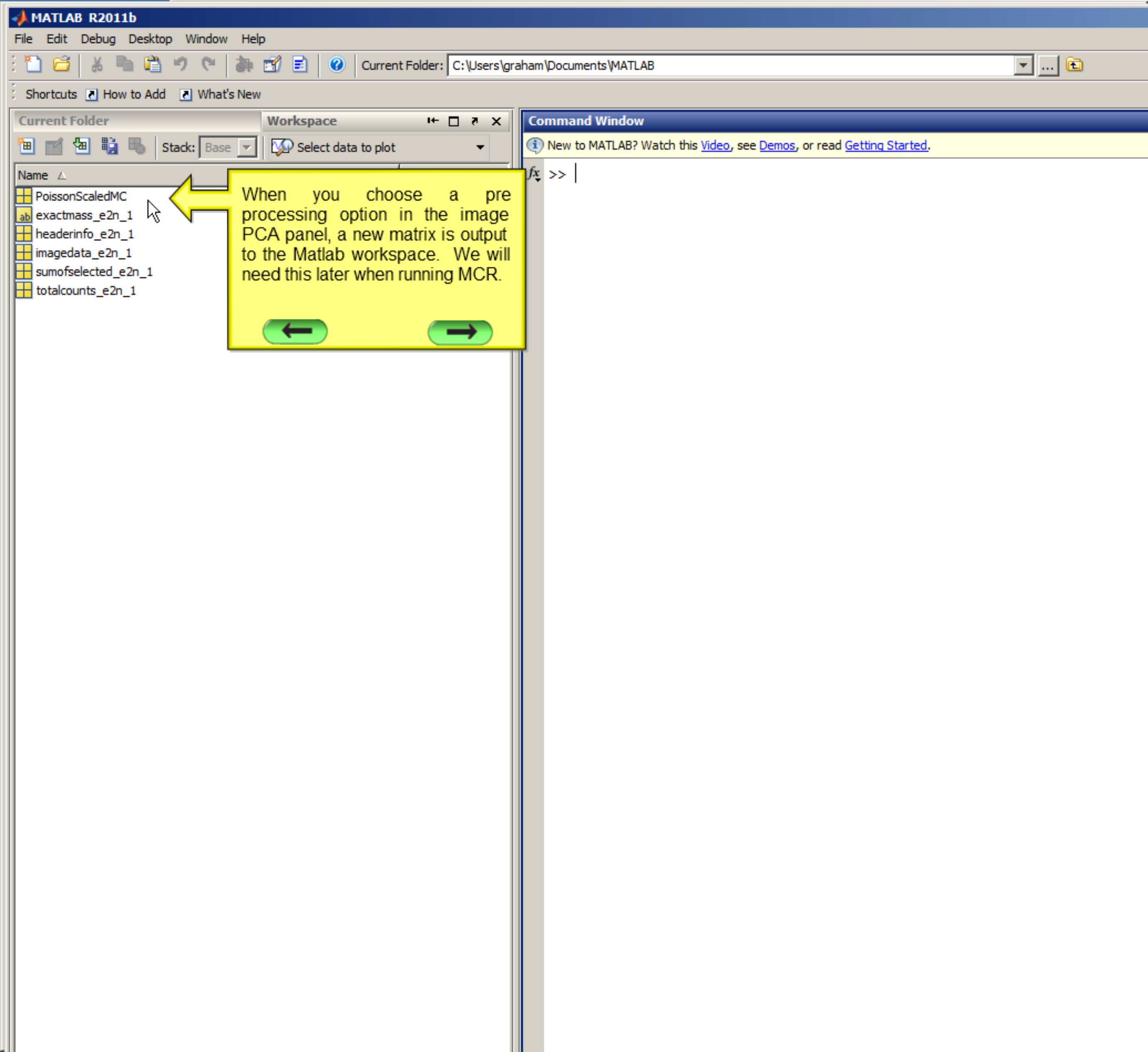
Save PCA Data

Next choose the type of pre-processing you would like to do on the data. You need to run MCR on the data that has been processed in the same way as the data used for PCA.

Here we wil choose to Poisson scale and then mean center the data.



Close Panel



Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

imagedata_e2n...

exactmass_e2n_1 ...

Load Selected Data

Image: **imagedata_e2n_1**

Variables **exactmass_e2n_1**


Data Preprocessing

Poisson Scaling & Mean Center

Run PCA

Press the 'Run PCA' button

PCA Summary		
PC#	%Var	%Vartotal



Name for scores matrix

Name for loadings matrix

Name for Variance matrix

of PCs to keep in model

Save PCA Data

Close Panel

Data Selection Panel

Name of Image Matrix

imagedata_e2n...

Name of Variable Matrix

exactmass_e2n_1 ...

Load Selected Data

Image: **imagedata_e2n_1**
Variables **exactmass_e2n_1**

Data Preprocessing

PoissonScaling & Mean Center

Run PCA

PCA Summary
PC# %Var %Vartotal

1	15.1	15.1
2	3.7	18.9
3	1	19.9
4	0.8	20.6
5	0.7	21.3
6	0.7	22
7	0.7	22.7
8	0.7	23.3
9	0.7	24
10	0.7	24.6

Name for scores matrix

Name for loadings matrix

Name for Variance matrix

of PCs to keep in model

Save PCA Data

PC #

1

Plot Scores and Loads

Split Pos/Neg S&L

Opens a separate
figure window

Browse all PCA plots

Opens a separate
figure window

☐ number PCs for Grid

Plot Multiple PCs in Grid

Opens a separate
figure window

Now let's look through the PCA results to see if we can determine how many components appear to be present in the sample.

Select the first PC and press 'Plot Scores and Loads'.



Close Panel

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

imagedata_e2n...

exactmass_e2n_1 ...

Load Selected Data

Image: **imagedata_e2n_1**

Variables: **exactmass_e2n_1**

Data Preprocessing

PoissonScaling & Mean Center

Run PCA

PCA Summary

From the PC1 scores plot it is apparent that there is a central spot, a bright background and some white spots. This would suggest maybe 3 components.

The negative loadings are indicative of DNA which should be on the spot (dark areas)



Name for loadings matrix

Name for Variance matrix

of PCs to keep in model

Save PCA Data

PC #

1

Plot Scores and Loads

Split Pos/Neg S&L

Opens a separate figure window

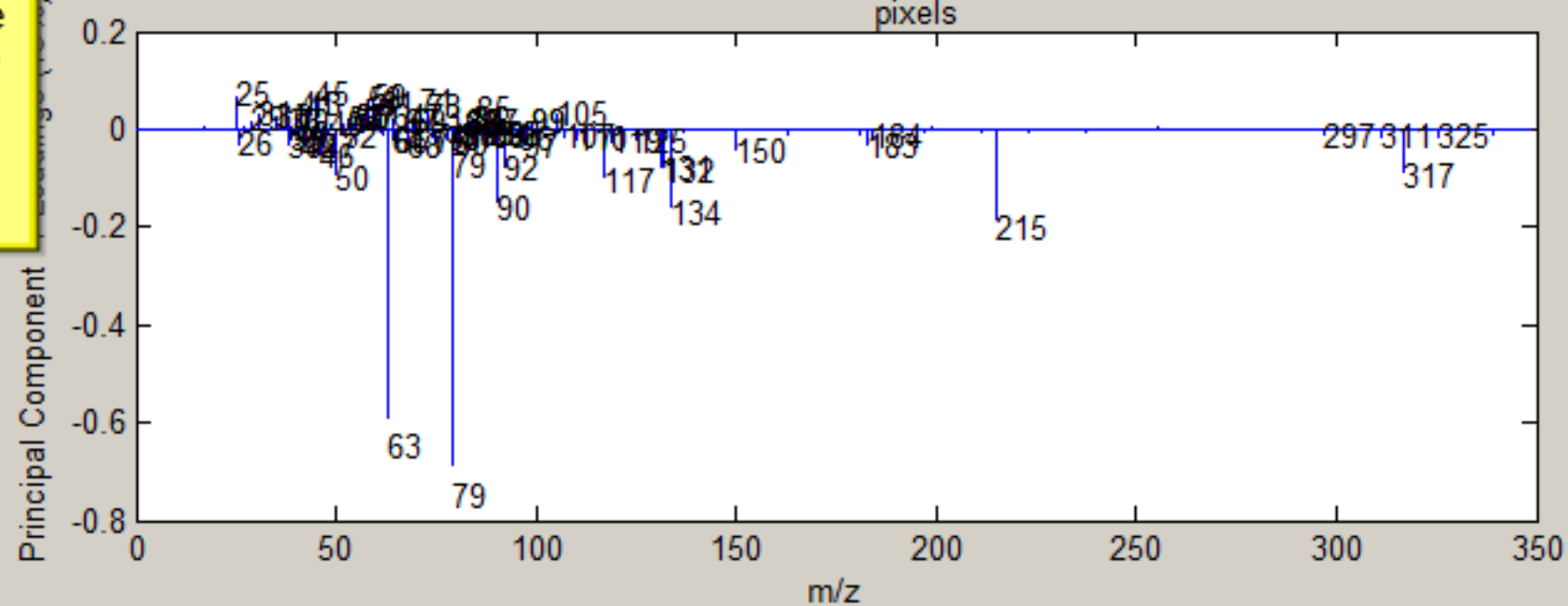
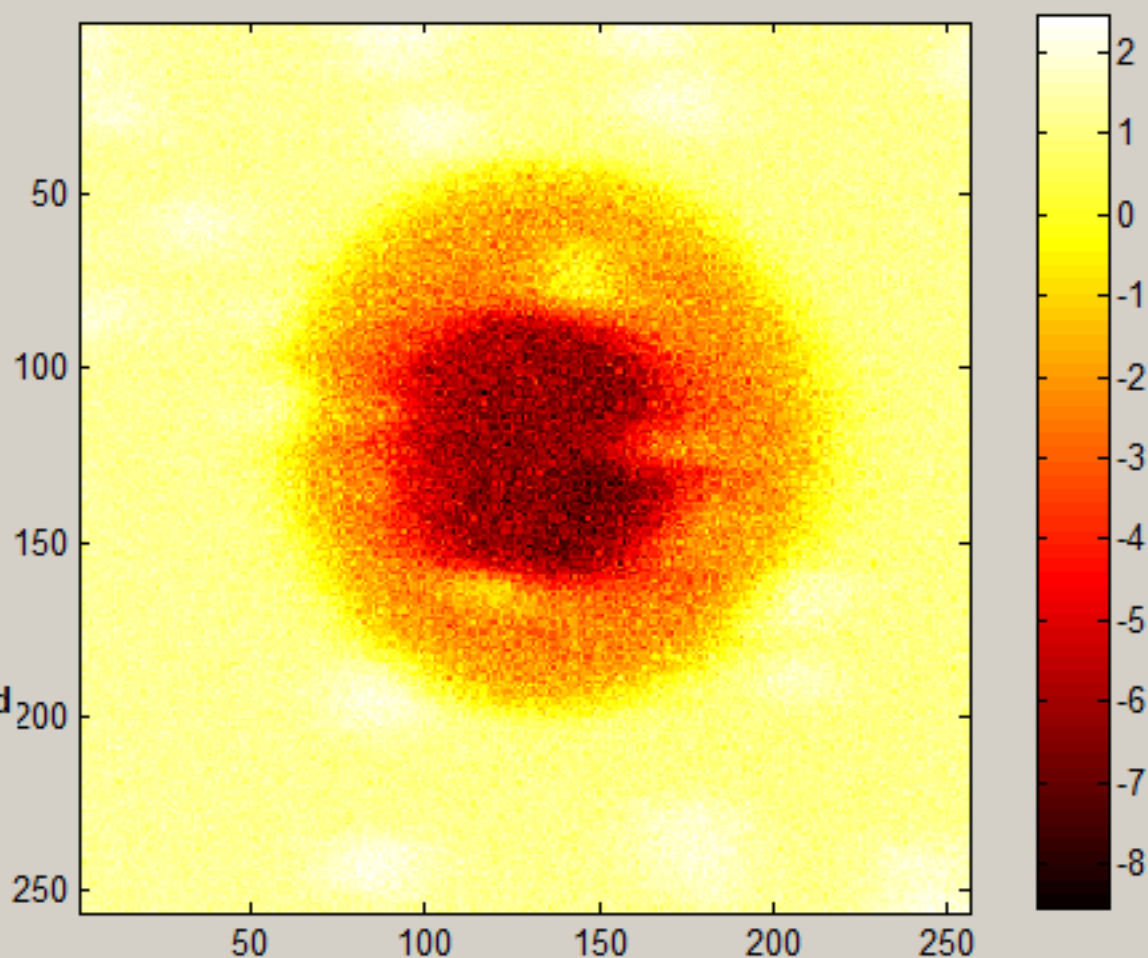
Browse all PCA plots

Opens a separate figure window

Number PCs for Grid

Plot Multiple PCs in Grid

Opens a separate figure window



Close Panel

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

imagedata_e2n...

exactmass_e2n_1 ...

Load Selected Data

Image: **imagedata_e2n_1**

Variables: **exactmass_e2n_1**

Data Preprocessing

PoissonScaling & Mean Center

Run PCA

PC #

2

Plot Scores and Loads

Split Pos/Neg S&L

Opens a separate figure window

Browse all PCA plots

Opens a separate figure window

PCs for Grid

Multiple PCs in Grid

Opens a separate figure window

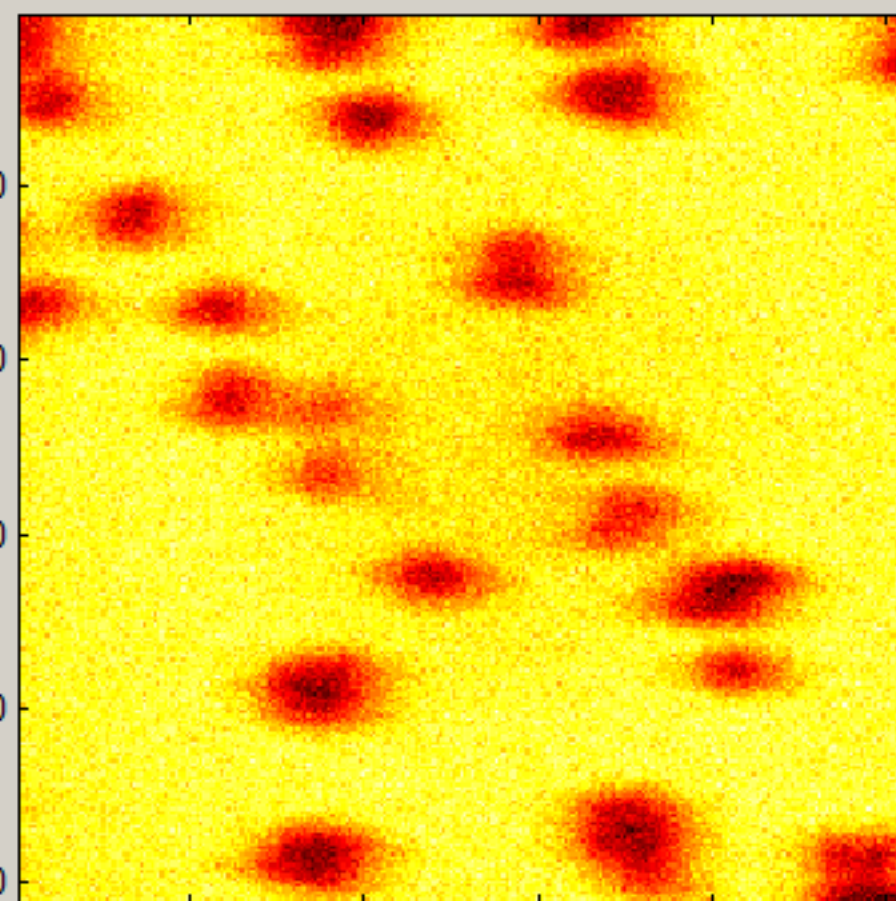
50

100

150

200

250



pixels

From the PC2 scores plot we see the spots again and the background. The loadings show the dark areas are showing peaks indicative of PEG (negative loadings) and the background is showing peaks typical of the silane linker on the substrate (positive loadings).



Name for scores matrix

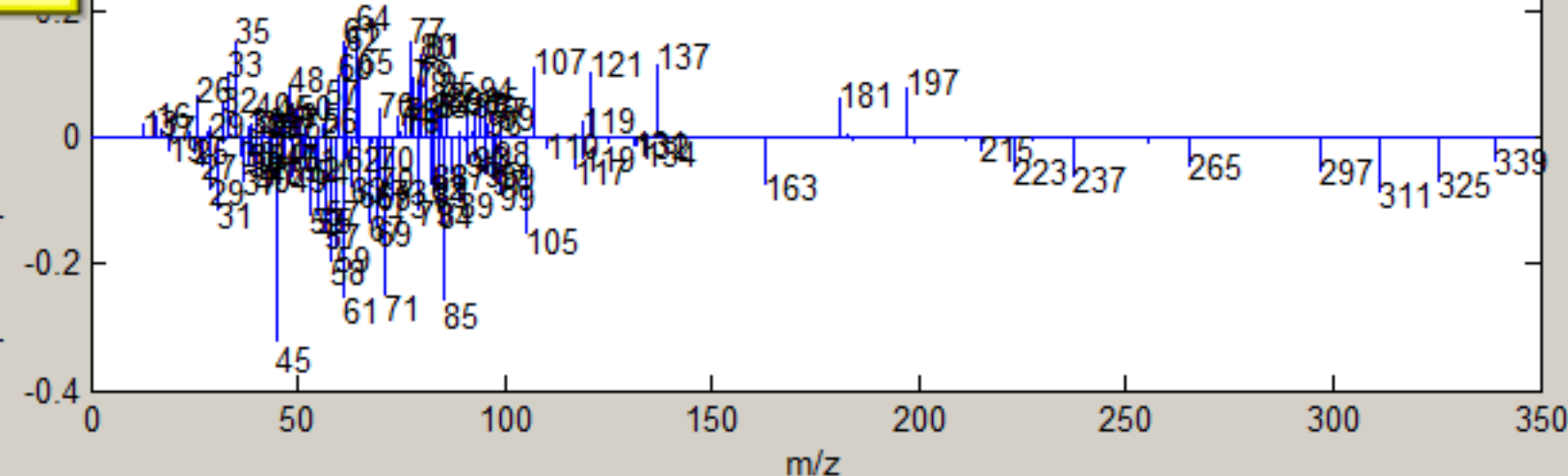
Name for loadings matrix

Name for Variance matrix

of PCs to keep in model

Save PCA Data

Principal Component 2 Loadings



Close Panel

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

imagedata_e2n...

exactmass_e2n_1 ...

Load Selected Data

Image: **imagedata_e2n_1**
Variables: **exactmass_e2n_1**

Data Preprocessing

PoissonScaling & Mean Center

Run PCA

PCA Summary

PC3 shows a gradient in the scores plot and some of the same peaks seen previously in PC2.

Other PCs show noise.



8	0.7	23.3
9	0.7	24
10	0.7	24.6

Name for scores matrix

Name for loadings matrix

Name for Variance matrix

of PCs to keep in model

Save PCA Data

PC #

3

Plot Scores and Loads

Split Pos/Neg S&L

Opens a separate figure window

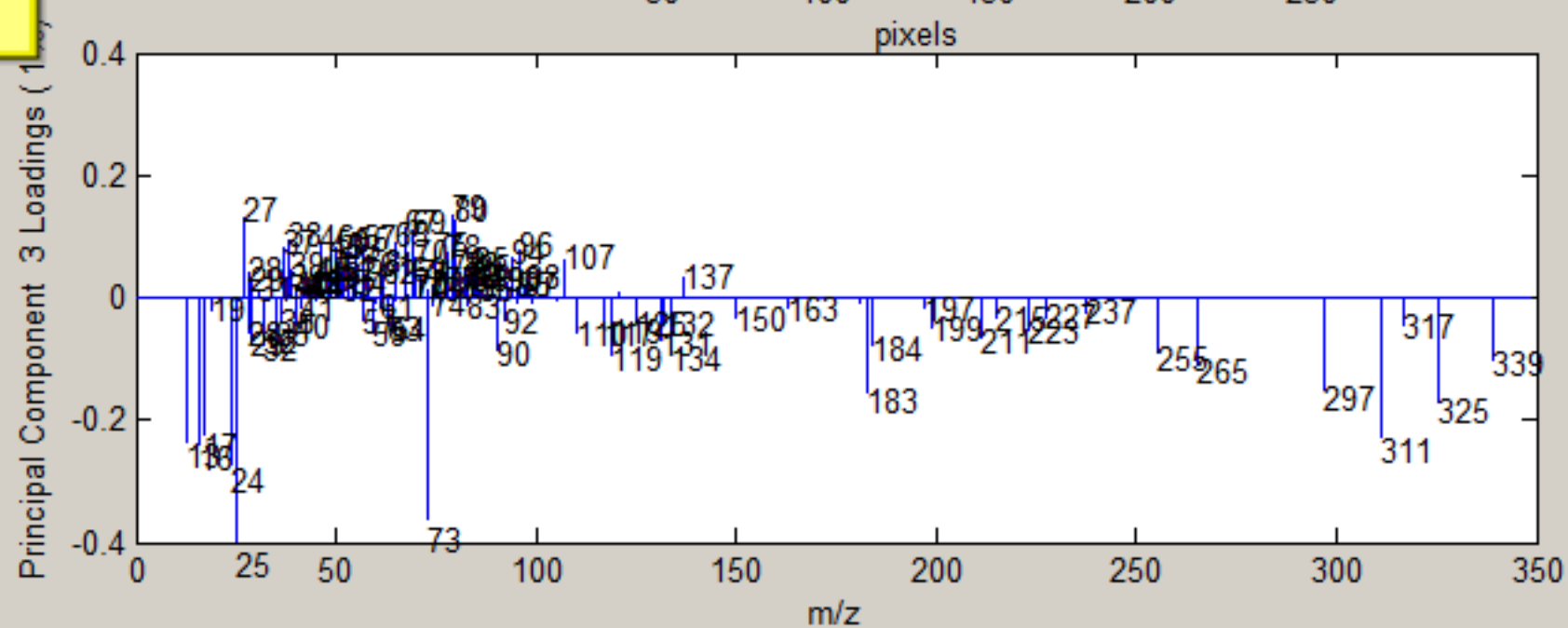
Browse all PCA plots

Opens a separate figure window

Number PCs for Grid

Plot Multiple PCs in Grid

Opens a separate figure window



Close Panel

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

imagedata_e2n...

exactmass_e2n_1 ...

Load Selected Data

Image: **imagedata_e2n_1**
Variables: **exactmass_e2n_1**

Data Preprocessing

PoissonScaling & Mean Center

Run PCA

PCA Summary
PC# %Var %Vartotal

PC#	%Var	%Vartotal
1	15.1	15.1
2	3.7	18.9
3	1	19.9
4	0.8	20.6
5	0.7	21.3
6	0.7	22
7	0.7	22.7
8	0.7	23.3
9	0.7	24
10	0.7	24.6

Name for scores matrix

scores

Name for loadings matrix

loads

Name for Variance matrix

var

of PCs to keep in model 3

Save PCA Data

PC #

3

Plot Scores and Loads

Split Pos/Neg S&L

Opens a separate figure window

Browse all PCA plots

Opens a separate figure window

number PCs for Grid

Plot Multiple PCs in Grid

Opens a separate figure window

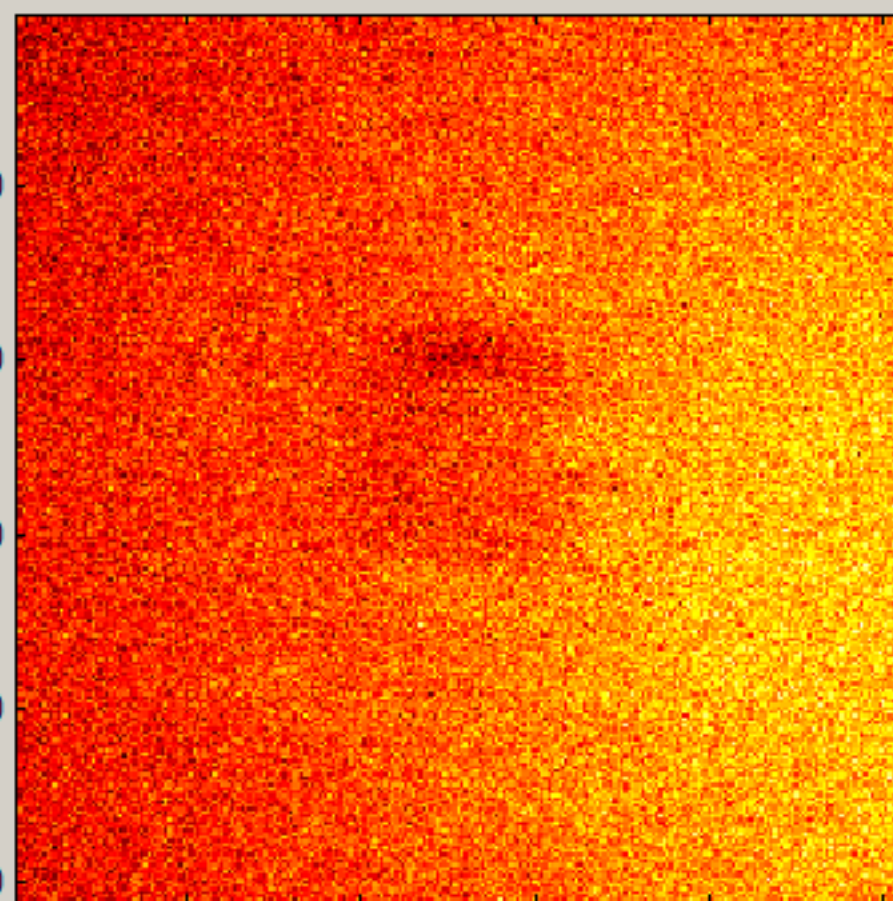
50

100

150

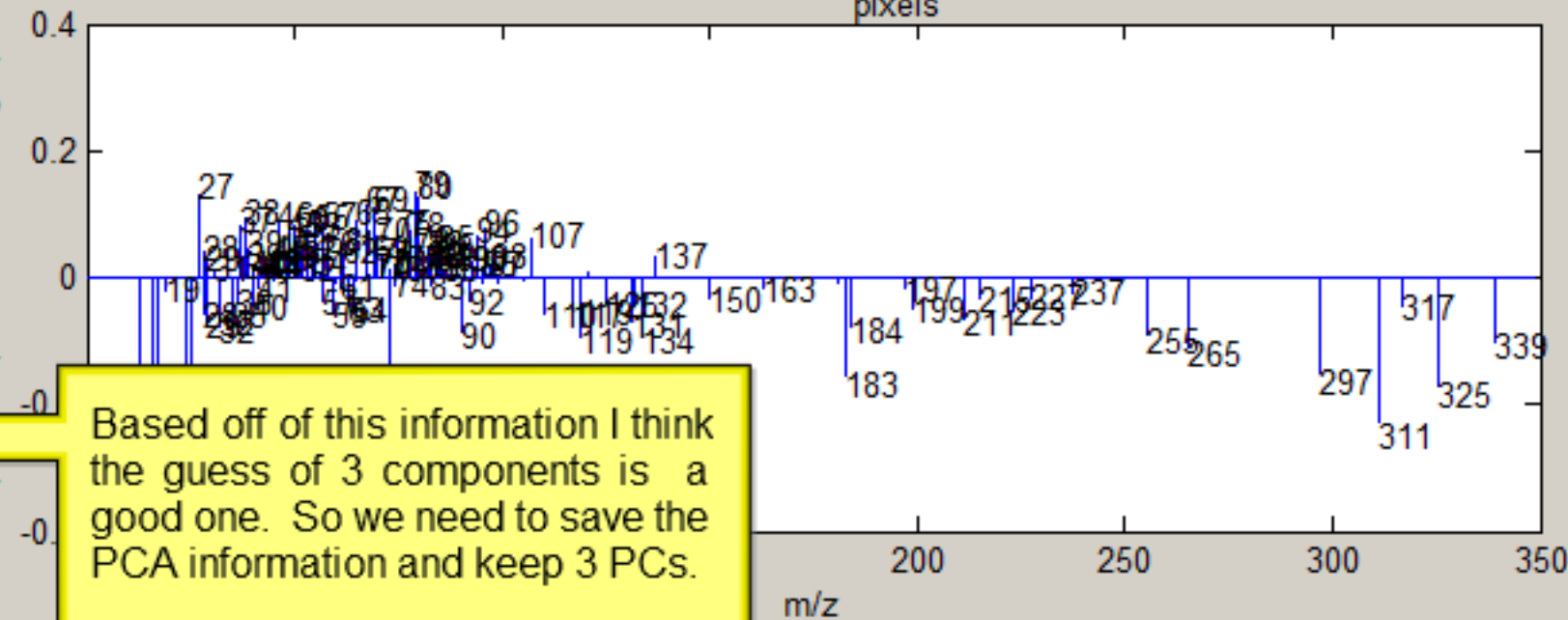
200

250



pixels

Component 3 Loadings (1%)



Based off of this information I think the guess of 3 components is a good one. So we need to save the PCA information and keep 3 PCs.

Fill in the boxes here and press the 'Save PCA Data' button.



Close Panel

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

imagedata_e2n...

exactmass_e2n_1 ...

Load Selected Data

Image: **imagedata_e2n_1**

Variables: **exactmass_e2n_1**

Data Preprocessing

PoissonScaling & Mean Center

Run PCA

PCA Summary

PC# %Var %Vartotal

1	15.1	15.1
2	3.7	18.9
3	1	19.9
4	0.8	20.6
5	0.7	21.3
6	0.7	22
7	0.7	22.7
8	0.7	23.3
9	0.7	24
10	0.7	24.6

Name for scores matrix

scores

Name for loadings matrix

loads

Name for Variance matrix

var

of PCs to keep in model 3

Save PCA Data

PC #

3

Plot Scores and Loads

Split Pos/Neg S&L

Opens a separate figure window

Browse all PCA plots

Opens a separate figure window

number PCs for Grid

Plot Multiple PCs in Grid

Opens a separate figure window

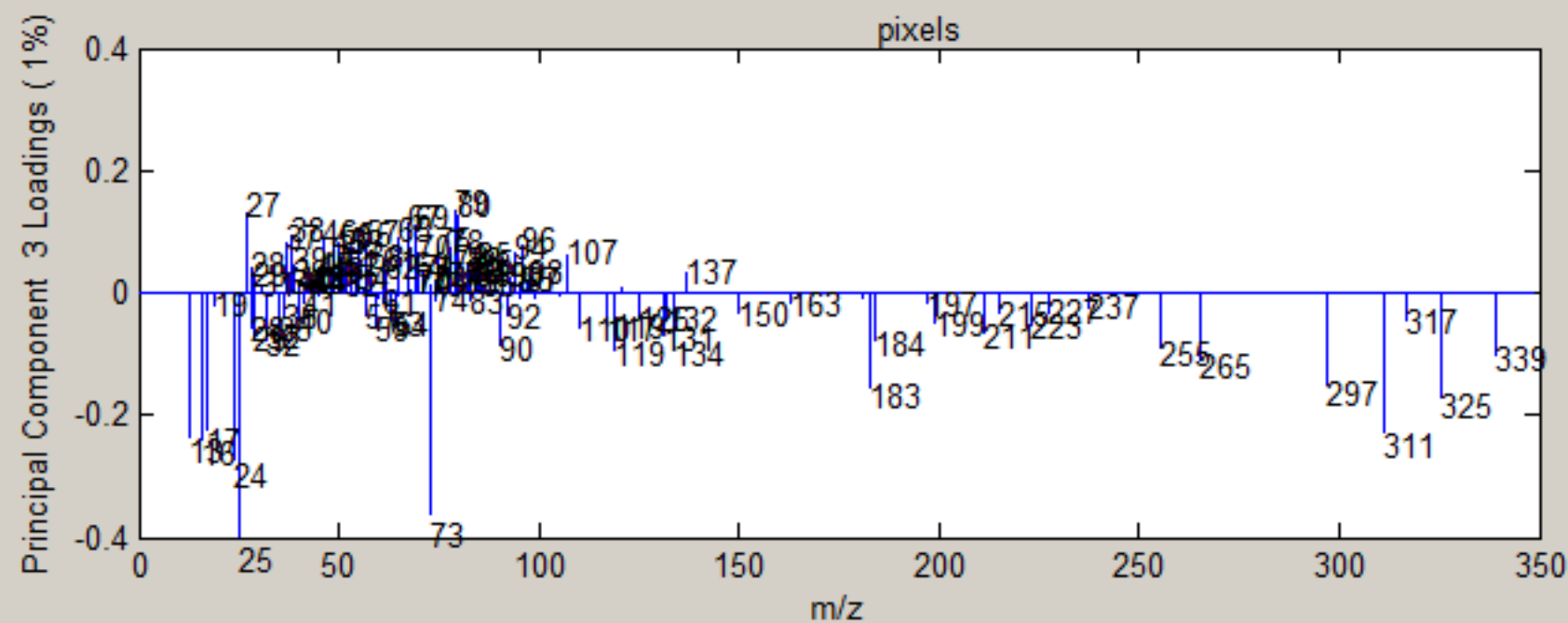
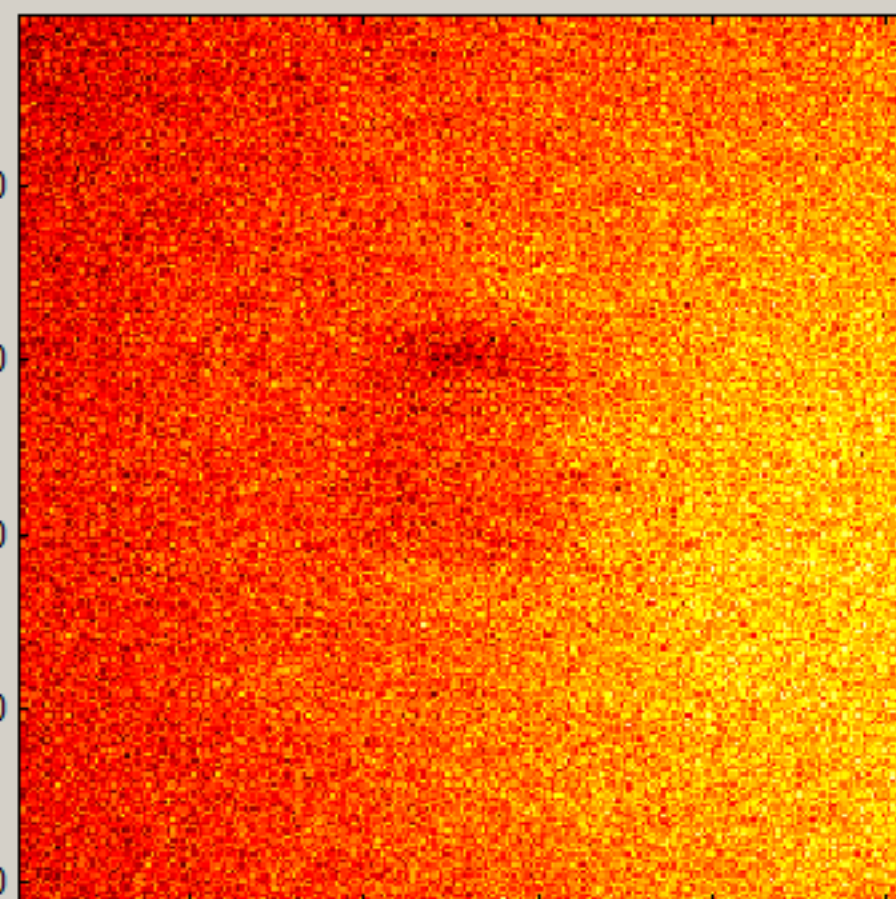
50

100

150

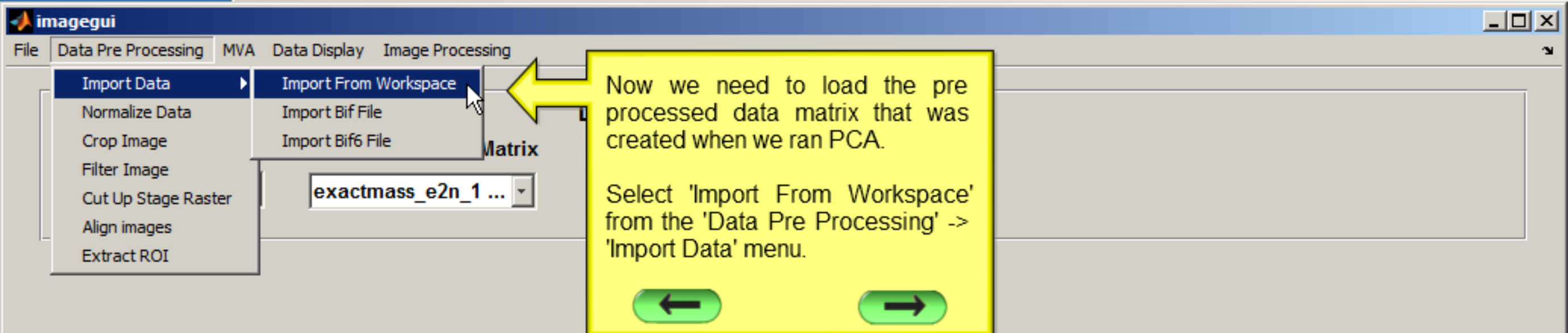
200

250



At this point we can close the PCA panel.

Close Panel



Data Selection Panel

Name of Image Matrix

imagedata_e2n...

Name of Variable Matrix

exactmass_e2n_1 ...

Import Data From Workspace

Press the "Get Variables" button to see a list of all variables in the workspace. Then select a variable and then press the appropriate button to load it into the proper list menu in the "Data Selection Panel".

Get Variables

Press 'Get Variables' to list the available data.



Add to Image Overlay List

MVA Data

Add to PCA Scores List

Add to PCA Loadings List

Add to PCA Variance List

Add to MAF Scores List

Add to MAF Loadings List

Add to MAF Variance List

Close Panel

Data Selection Panel

Name of Image Matrix

imagedata_e2n...

Name of Variable Matrix

exactmass_e2n_1

Import Data From Workspace

Press the "Get Variables" button to see a list of all variables in the workspace. Then select a variable and then press the appropriate button to load it into the proper list menu in the "Data Selection Panel".

Get Variables

PCA_loads
PCA_scores
PCA_var
PoissonScaledMC
exactmass_e2n_1
headerinfo_e2n_1
imagedata_e2n_1
sumofselected_e2n_1
totalcounts_e2n_1

Data

Add to Image List

Add to Variable List

Add to Image Overlay List

MVA Data

Add to PCA Scores List

Add to PCA Loadings List

Add to PCA Variance List

Add to MAF Scores List

Add to MAF Loadings List

Add to MAF Variance List

Close Panel

Select the pre processed data matrix and press 'Add to Image List'.



Data Selection Panel

Name of Image Matrix

imagedata_e2n...

Name of Variable Matrix

exactmass_e2n_1

Import Data From Workspace

Press the "Get Variables" button to see a list of all variables in the workspace. Then select a variable and then press the appropriate button to load it into the proper list menu in the "Data Selection Panel".

imagedetailgui

Please fill in the information below

Name of Total counts matrix

Choose one...

Name of sum of selected matrix

Choose one...

☒ I do not need Total or Sum Images

Close

Data

Add to Image List

Add to Variable List

Add to Image Overlay List

MVA Data

Add to MAF Scores List

Add to MAF Loadings List

Add to MAF Variance List

Close Panel

We don't need the Total counts or Sum images so check this box.

Data Selection Panel

Name of Image Matrix

imagedata_e2n...

Name of Variable Matrix

exactmass_e2n_1

Import Data From Workspace

Press the "Get Variables" button to see a list of all variables in the workspace. Then select a variable and then press the appropriate button to load it into the proper list menu in the "Data Selection Panel".

imagedetailgui

Please fill in the information below

Name of Total counts matrix

Choose one...

Name of sum of selected matrix

Choose one...

☒ I do not need Total or Sum Images

Close

Close this dialog box.

Data

Add to Image List

Add to Variable List

Add to Image Overlay List

MVA Data

Add to PCA Scores List

Add to MAF Loadings List

Add to MAF Variance List

Close Panel

Data Selection Panel

Name of Image Matrix

imagedata_e2n...

Name of Variable Matrix

exactmass_e2n_1

Import Data From Workspace

Press the "Get Variables" button to see a list of all variables in the workspace. Then select a variable and then press the appropriate button to load it into the proper list menu in the "Data Selection Panel".

Get Variables

PCA_loads
PCA_scores
PCA_var
PoissonScaledMC
exactmass_e2n_1
headerinfo_e2n_1
imagedata_e2n_1
sumofselected_e2n_1
totalcounts_e2n_1

Data

Add to Image List

Add to Variable List

Add to Image Overlay List

MVA Data

Add to PCA Scores List

Add to PCA Loadings List

Add to PCA Variance List

Add to MAF Scores List

Add to MAF Loadings List

Add to MAF Variance List

Close Panel

And close this panel.



Data Selection Panel

Name of Image Matrix

imagedata_e2n...

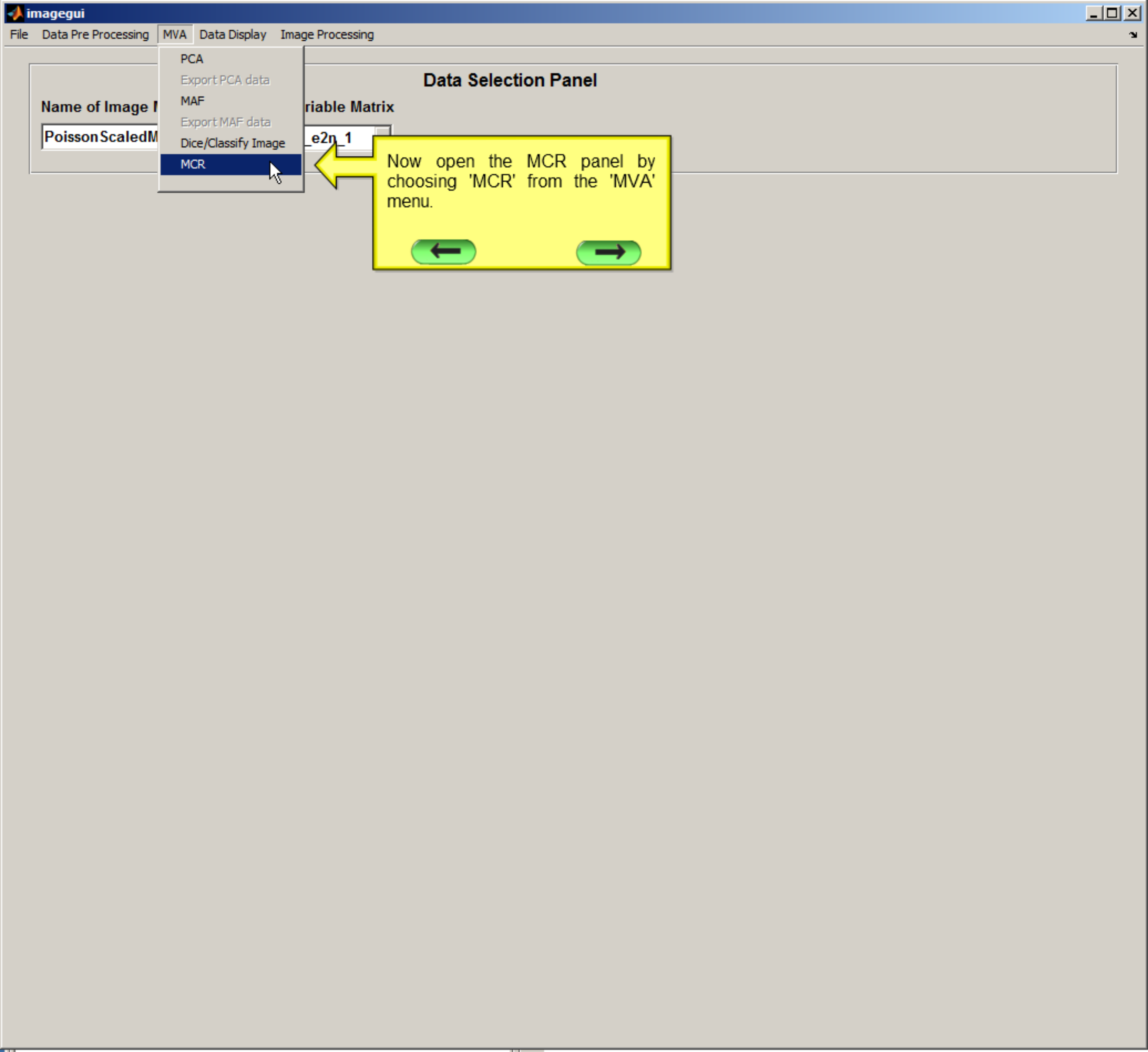
- Select Data
- imagedata_e2n_1
- Poisson ScaledMC

Name of Variable Matrix

exactma

Make sure the pre processed data is selcted from the 'Name of Image Matrix' drop down menu.





Name of Image I

Poisson Scaled M

PCA

Export PCA data

MAF

Export MAF data

Dice/Classify Image

MCR

Variable Matrix

e2n_1

Data Selection Panel

Now open the MCR panel by
choosing 'MCR' from the 'MVA'
menu.



Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

PoissonScaledM...

exactmass_e2n_1

Scores

Loadings

Variance

Select Scores

Select Loadings

Select Variance

Load Selected Data

Image:

none

Variables

none

Press the 'Load Selected Data' button to load the data into the panel.

inter

Tol.

You must have the MCR-ALS toolbox installed to use this panel

MCR Code written by
Roma Tauler and Anna de Juan, 1999
Chemometrics and Solution
Equilibria group
University of Barcelona
Department of Analytical Chemistry
Diagonal 647, Barcelona 08028
e-mail roma@quimio.qui.ub.es

This implementation of MCR uses the following defaults:

- Non negativity for components and spectra
- fast non linear least squares (fnls)
- no closure

Depending on your data set it can take some time to run MCR. WAIT until you see a plot of the first MCR component to proceed.

Run MCR

Save MCR Results

Visit MCR-ALS Website

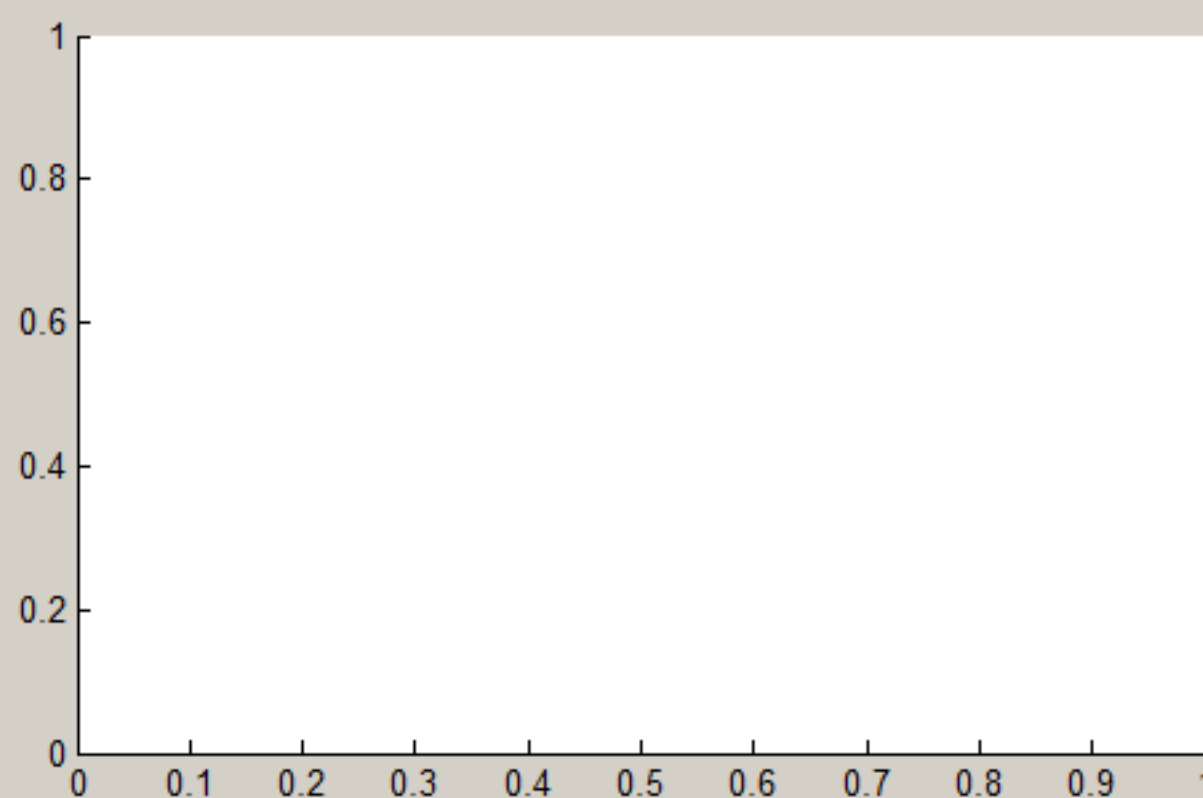
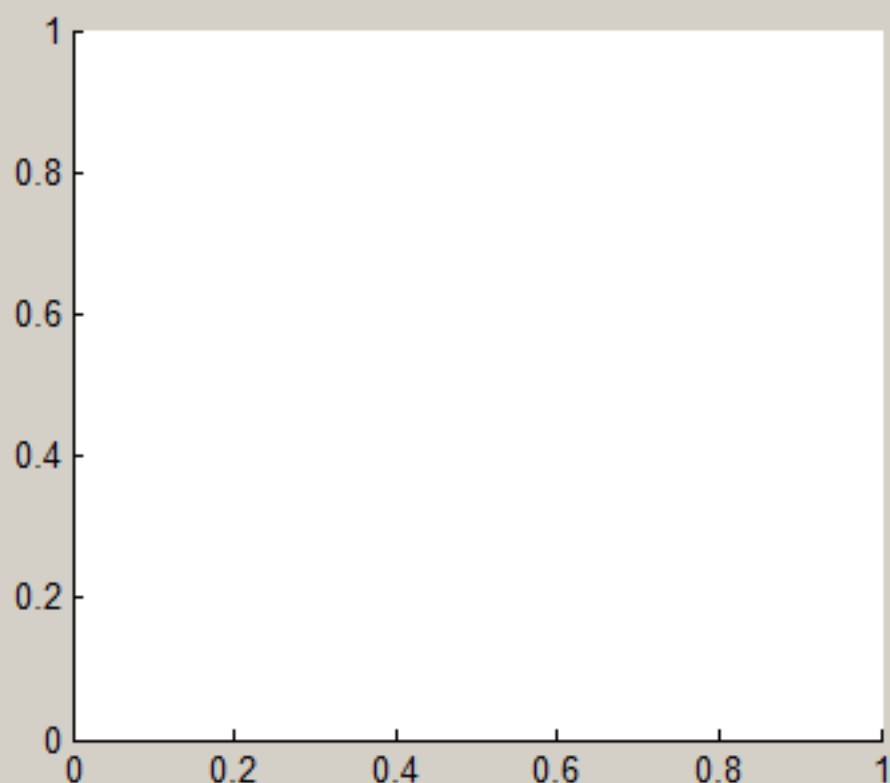
Choose component #

Plot Sel Comp

Plot All Comp

Save Fig

Make Ext



Close panel

Data Selection Panel

Name of Image Matrix

PoissonScaledM...

Name of Variable Matrix

exact

Scores

Select Scores ...

Select Scores

PCA_scores

Loadings

Select Loadings

Variance

Select Variance

Select the scores matrix you saved previously.

Load Selected Data

Image: PoissonScaledM...

Variables: exactmass_e2n_1

Init Est:

none

Tol.

You must have the MCR-ALS toolbox installed to use this panel

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Department of Analytical Chemistry
Diagonal 647, Barcelona 08028
e-mail roma@quimio.qui.ub.es

Visit MCR-ALS Website

This implementation of MCR uses the following defaults:

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- fast non linear least squares (fnls)
- no closure

Depending on your data set it can take some time to run MCR. WAIT until you see a plot of the first MCR component to proceed.

Run MCR

Save MCR Results

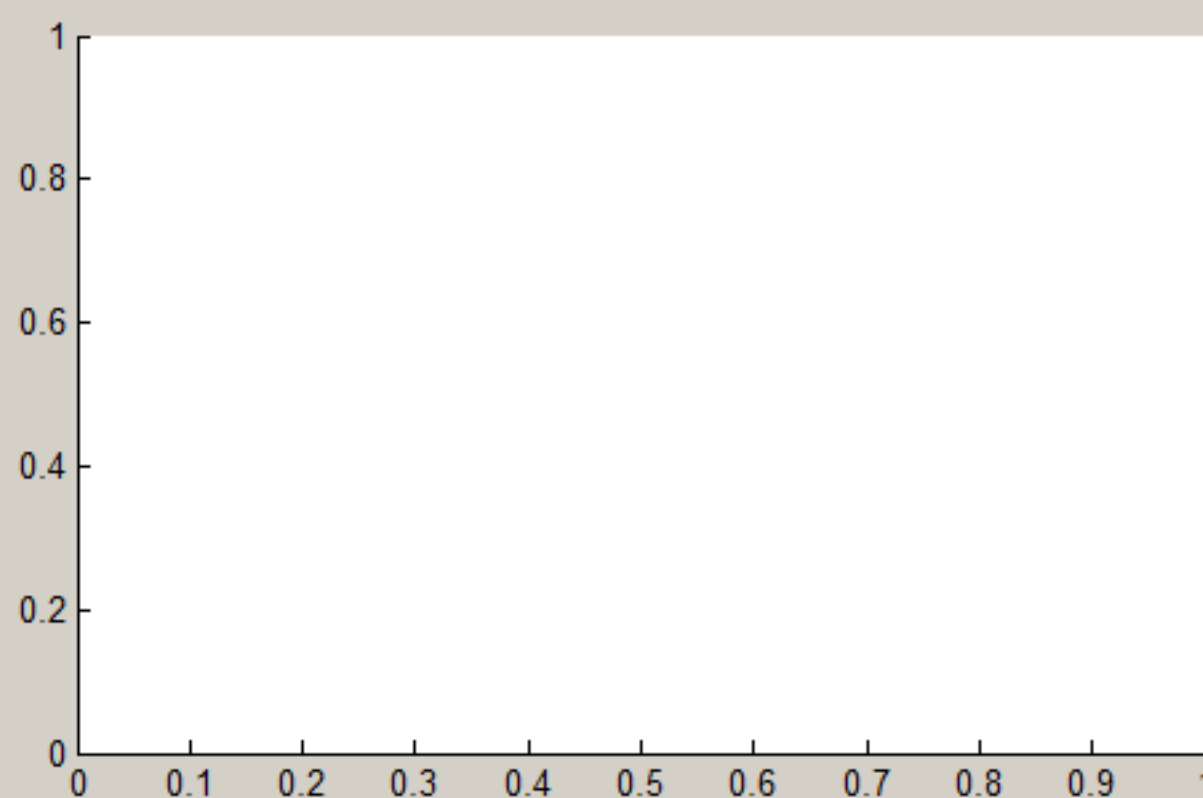
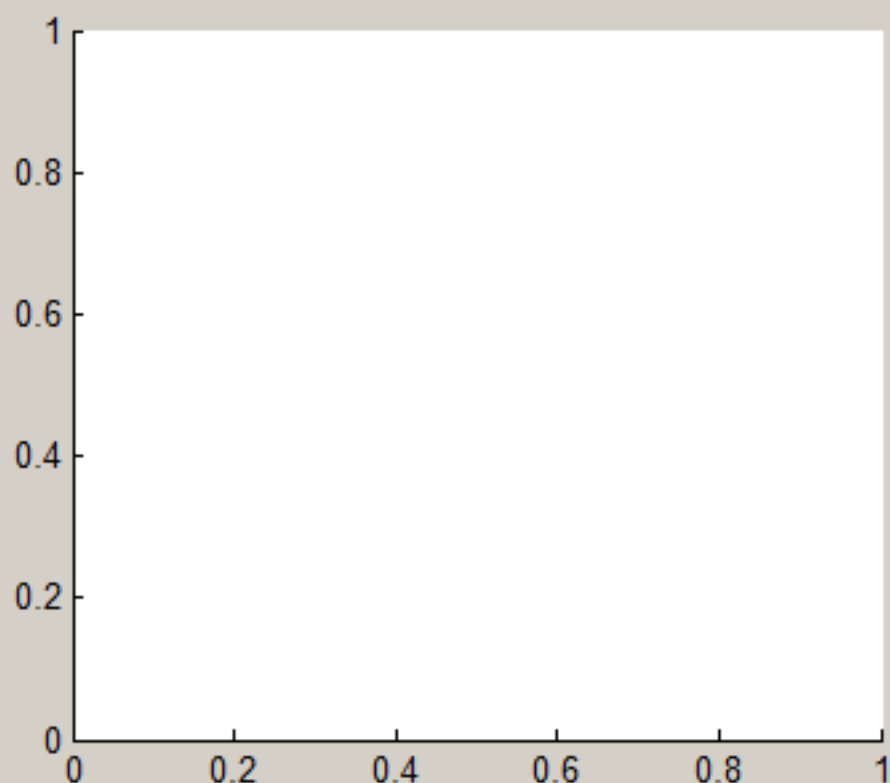
Choose component #

Plot Sel Comp

Plot All Comp

Save Fig

Make Ext



Close panel

Data Selection Panel

Name of Image Matrix

PoissonScaledM...

Name of Variable Matrix

exactmass_e2n_1

Scores

PCA_scores ...

Loadings

Select Loadings

Variance

Select Variance

Load Selected Data

Image: PoissonScaledMC

Variables exactmass_e2n_1

Load Selected Scores

or use:

Init Est:

none

This implementation of MCR uses the following defaults:

- Non negativity for components and spectra
- fast non linear least squares (fnls)
- no closure

Depending on your data set it can take some time to run MCR. WAIT until you see a plot of the first MCR component to proceed.

Run MCR

Save MCR Res

Visit MCR-ALS Website

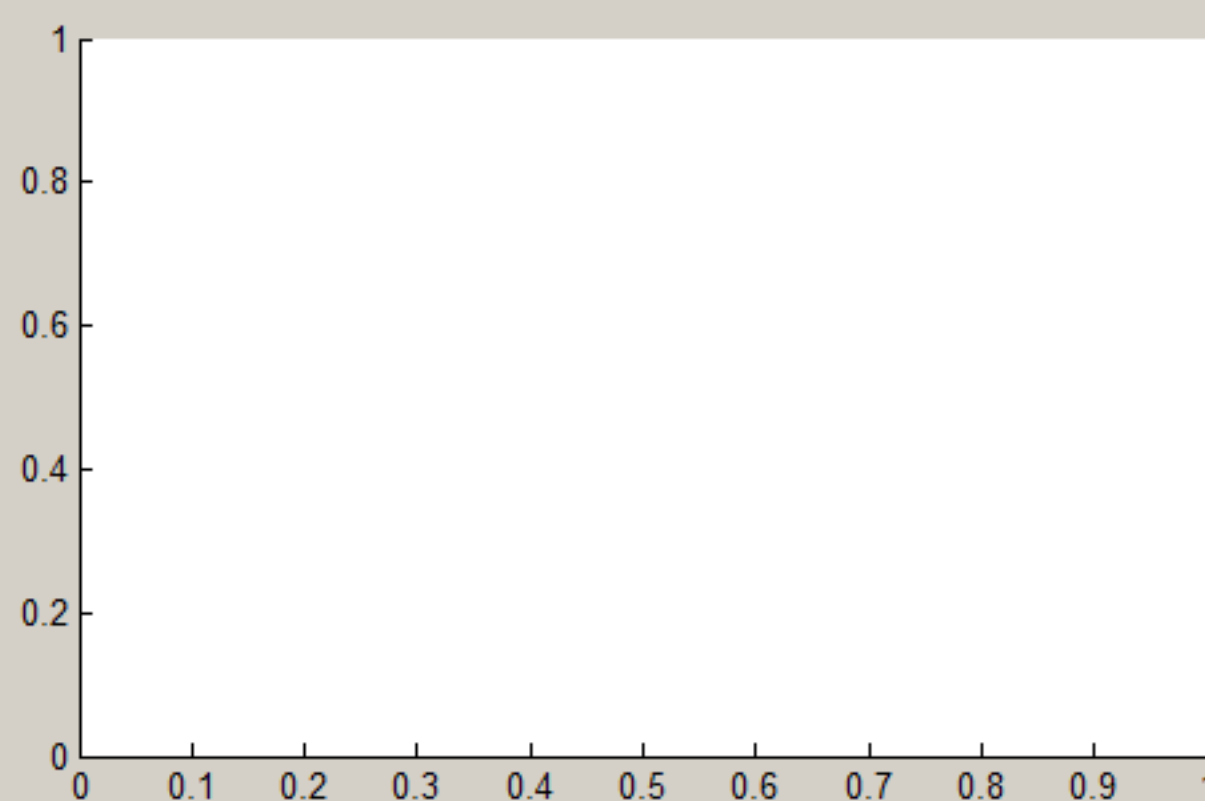
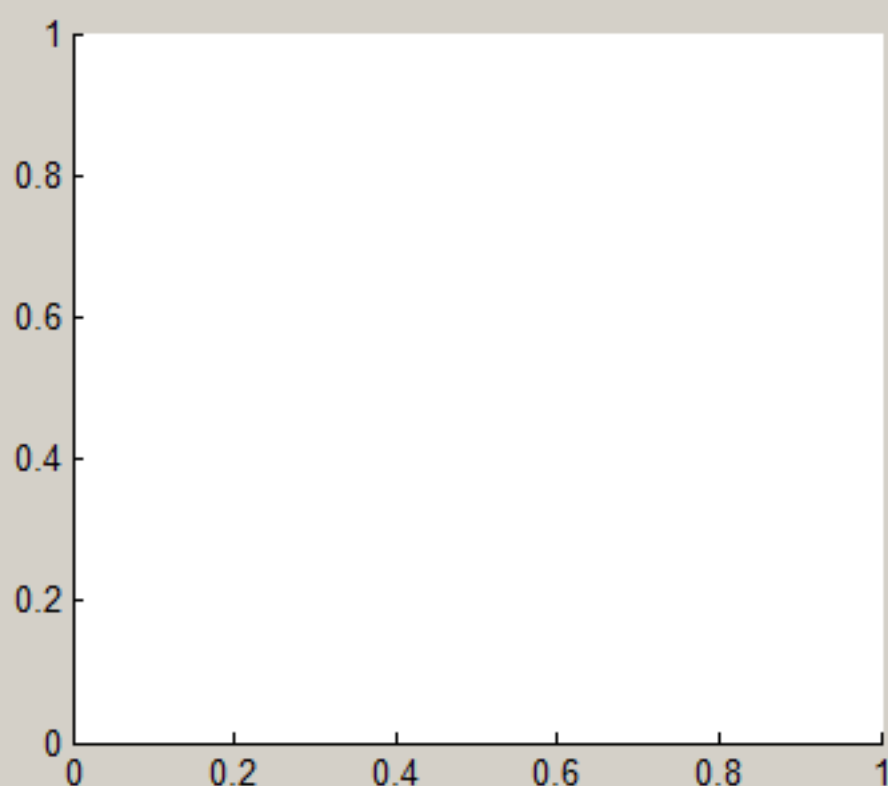
Choose component #

Plot Sel Comp

Plot All Comp

Save Fig

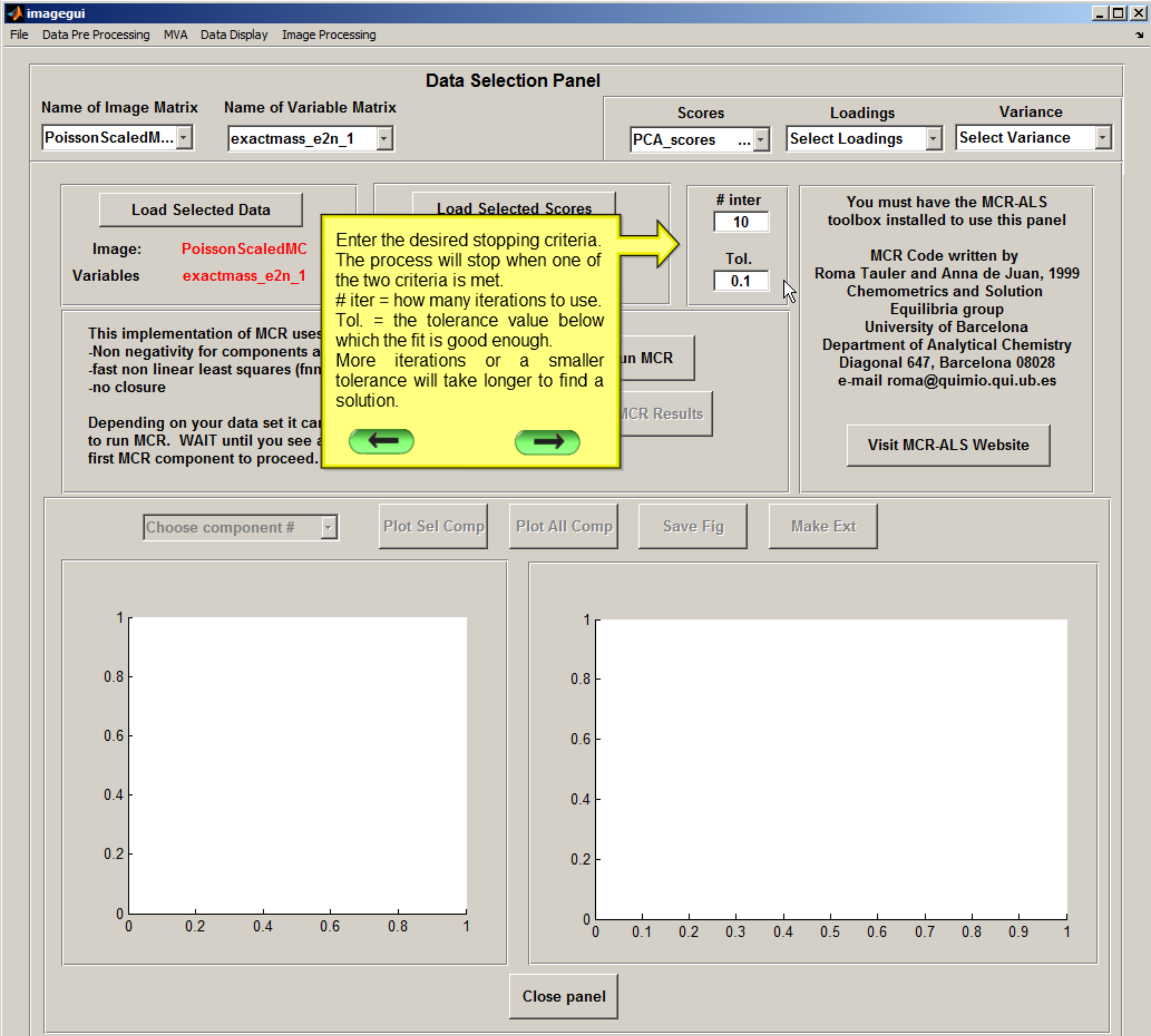
Make Ext



Close panel

The press the 'Load Selected Scores' button.

You can use any matrix you want as the initial guess. To use a non-scores matrix, enter the name of the matrix in the box below. That matrix must be within the active Matlab workspace.



Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

PoissonScaledM...

exactmass_e2n_1

Scores

PCA_scores ...

Loadings

Select Loadings

Variance

Select Variance

Load Selected Data

Image: **PoissonScaledMC**
Variables **exactmass_e2n_1**

Load Selected Scores

or use: Init Est: **PCA_scores**

iter

10

Tol.

0.1

You must have the MCR-ALS
toolbox installed to use this panel

MCR Code written by
Roma Tauler and Anna de Juan, 1999
Chemometrics and Solution
Equilibria group
University of Barcelona

This implementation of MCR uses the following defaults:

- Non negativity for components and spectra
- fast non linear least squares (fnls)
- no closure

Depending on your data set it can take some time
to run MCR. WAIT until you see a plot of the
first MCR component to proceed.

Run MCR

Save MCR Results

Press the 'Run MCR' button to start
MCR processing.

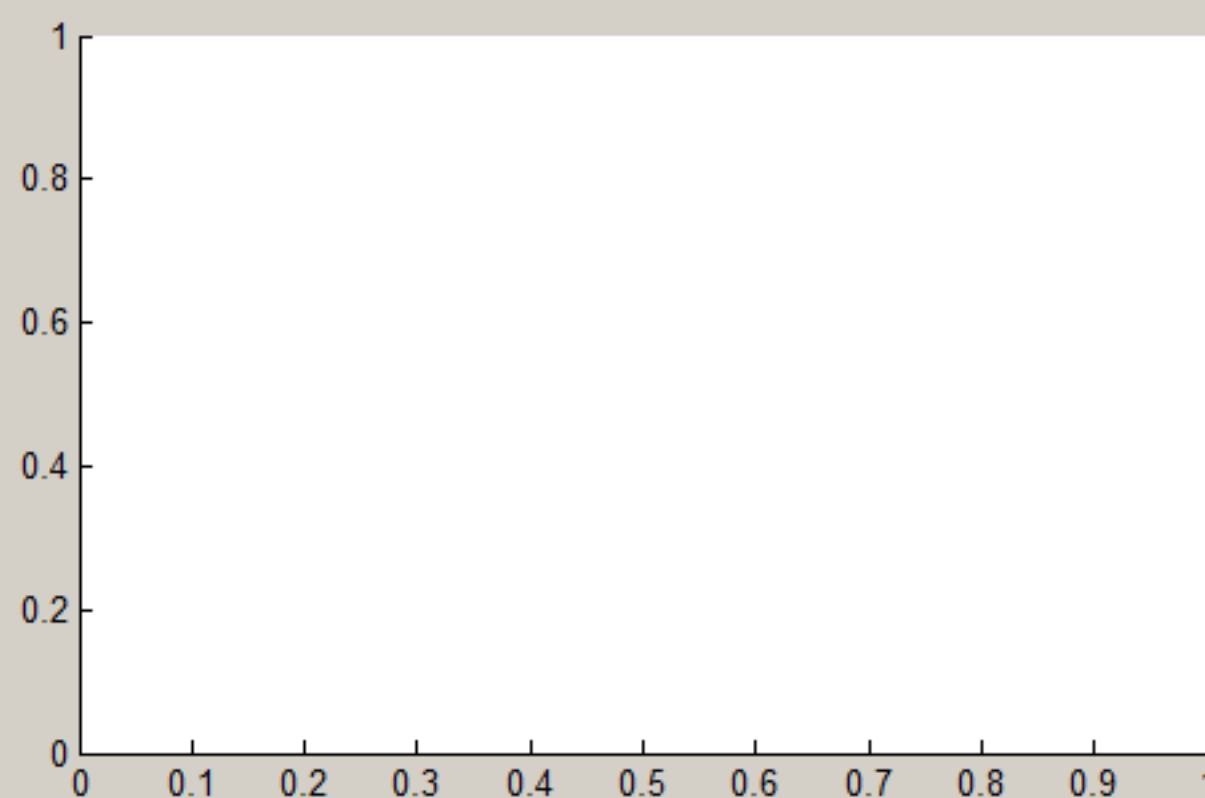
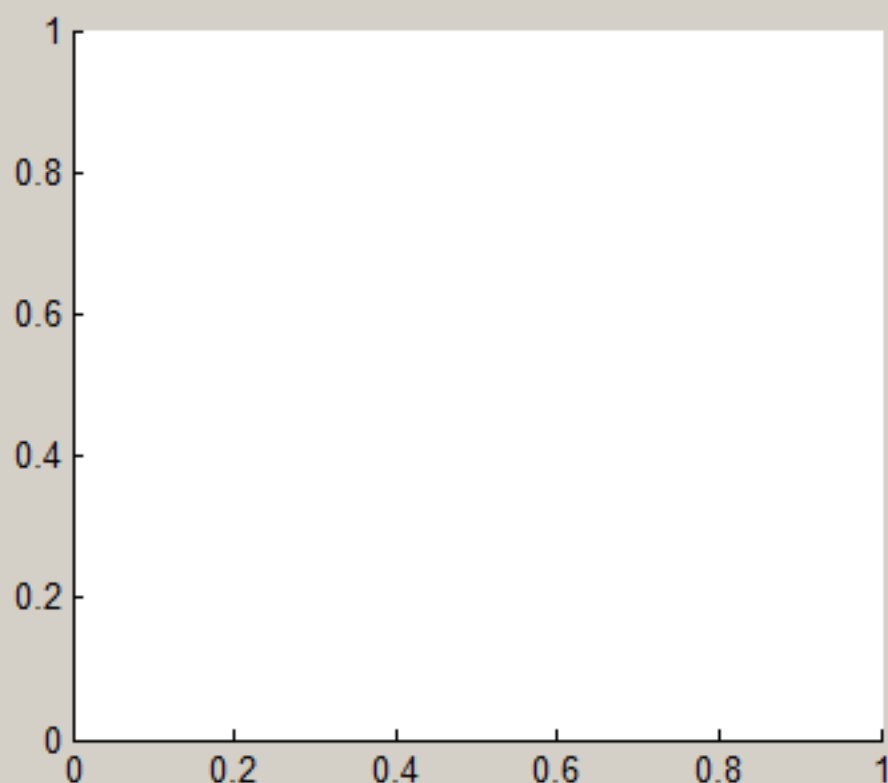
Choose component #

Plot Sel Comp

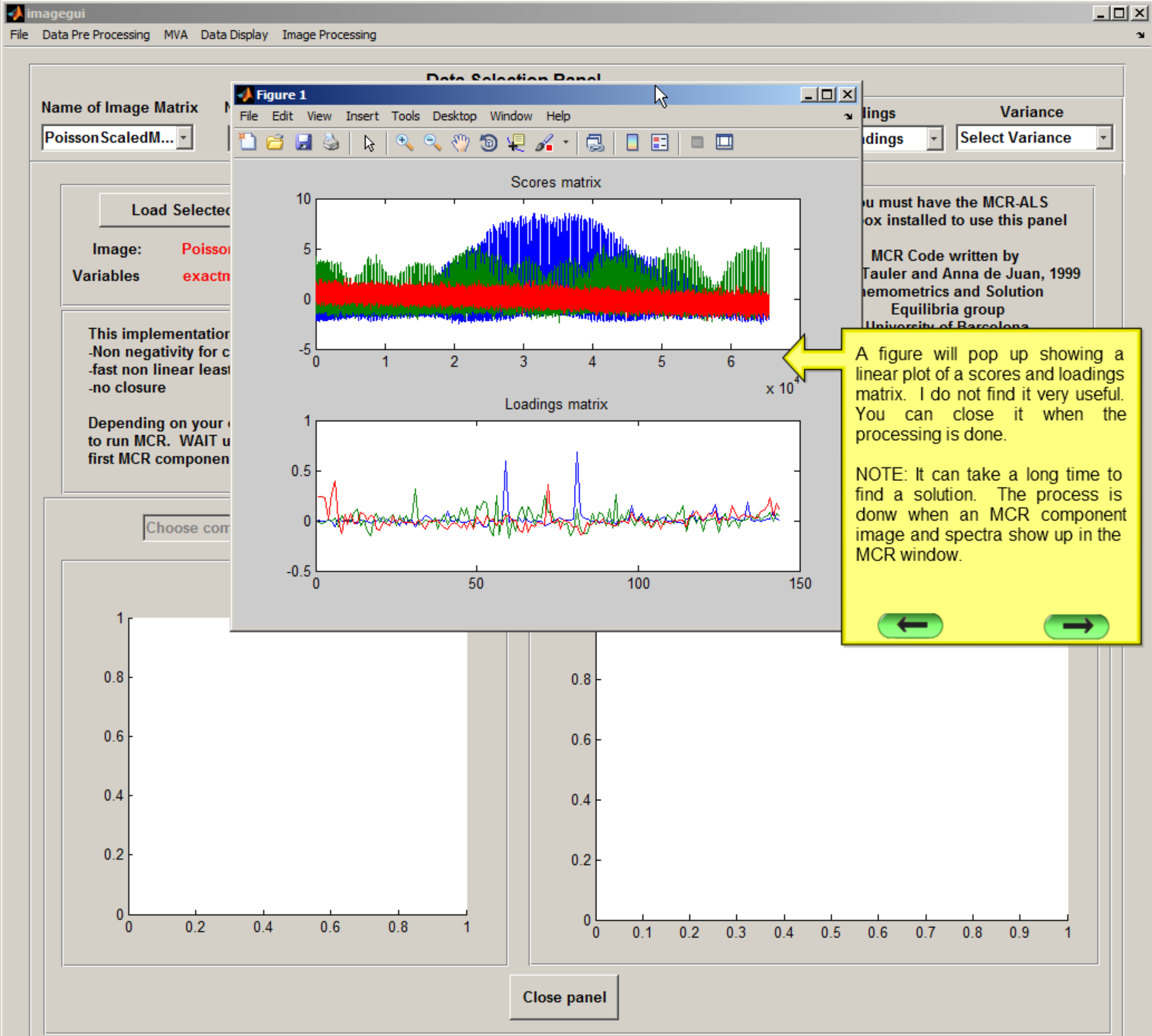
Plot All Comp

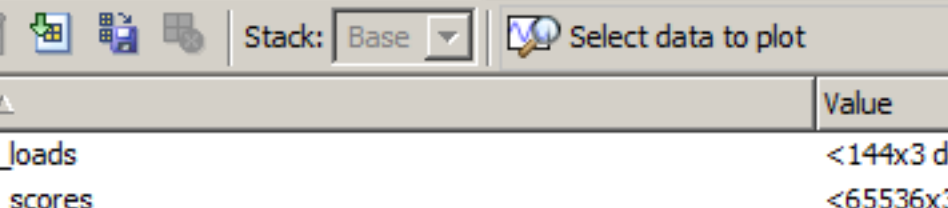
Save Fig

Make Ext



Close panel





The screenshot shows the MATLAB workspace window. The 'Current Folder' tab is active, displaying icons for various file types. The 'Stack' is set to 'Base'. The 'Select data to plot' button is visible. The workspace table lists the following variables:

Name	Value
PCA_loads	<144x3 double>
PCA_scores	<65536x3 double>
PCA_var	[15.1403; 3.7404; 0. ...]
PoissonScaledMC	<65536x144 double>
exactmass_e2n_1	<144x8 char>
headerinfo_e2n_1	
imagedata_e2n_1	
sumofselected_e2n_1	
totalcounts_e2n_1	

A yellow callout box with a pointer to the 'exactmass_e2n_1' variable contains the text: "While the computer is working on the solution, this information will be output within the workspace. It is a 144x8 character array."

While the computer is working on the solution, this information will be output within the workspace. It shows a summary of the fitting procedure.

Command Window

 New to MATLAB? Watch this [Video](#), see [Demos](#), or read [Getting Started](#).

ITERATION 1

```
Sum of squares respect PCA reprod. = 403288.0538
```

Old sigma = 1446.3993 -----> New sigma = 0.20672

Sigma respect experimental data = 0.46946

FITTING IS IMPROVING !!!

Change in sigma (%) = 699583.6453

```
Fitting error (lack of fit, lof) in % (PCA) = 98.5147
```

Fitting error (lack of fit, lof) in % (exp) = 99.7084

Percent of variance explained (r^2) is 0.58239

 $f_{x_{\downarrow}} \gg$

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

PoissonScaledM...

exactmass_e2n_1

Scores

Loadings

Variance

PCA_scores ...

Select Loadings

Select Variance

Load Selected Data

Load Selected Scores

inter

10

Tol.

0.1

You must have the MCR-ALS toolbox installed to use this panel

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University of Barcelona
Department of Analytical Chemistry
Diagonal 647, Barcelona 08028
e-mail roma@quimio.qui.ub.es

Visit MCR-ALS Website

This implementation of MCR uses the following defaults:

- Non negativity for components and spectra
- fast non linear least squares (fnls)
- no closure

Depending on your data set it can take some time to run MCR. WAIT until you see a plot of the first MCR component to proceed.

Run MCR

Save MCR Results

1

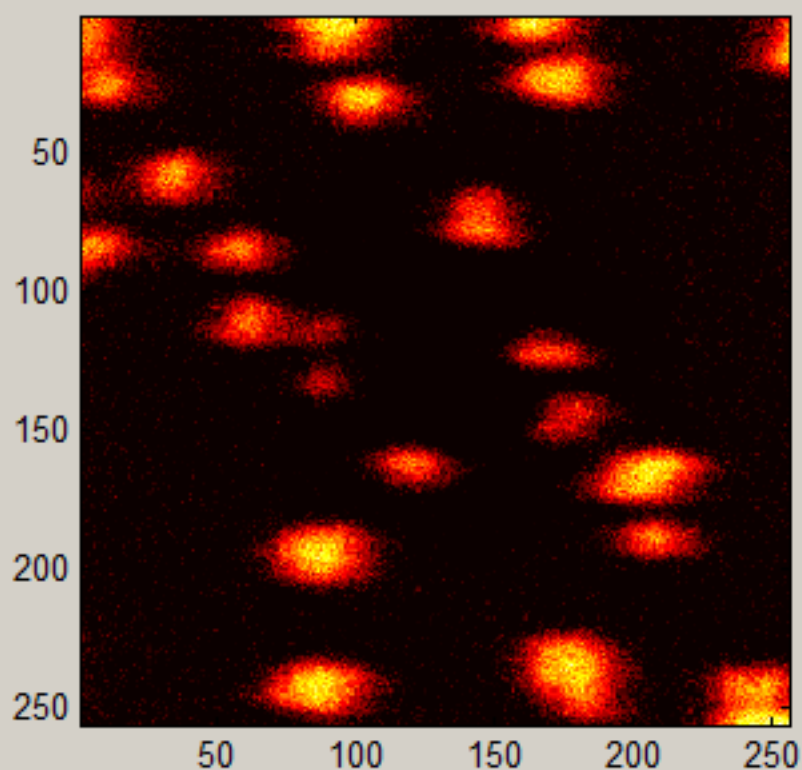
Plot Sel Comp

Plot All Comp

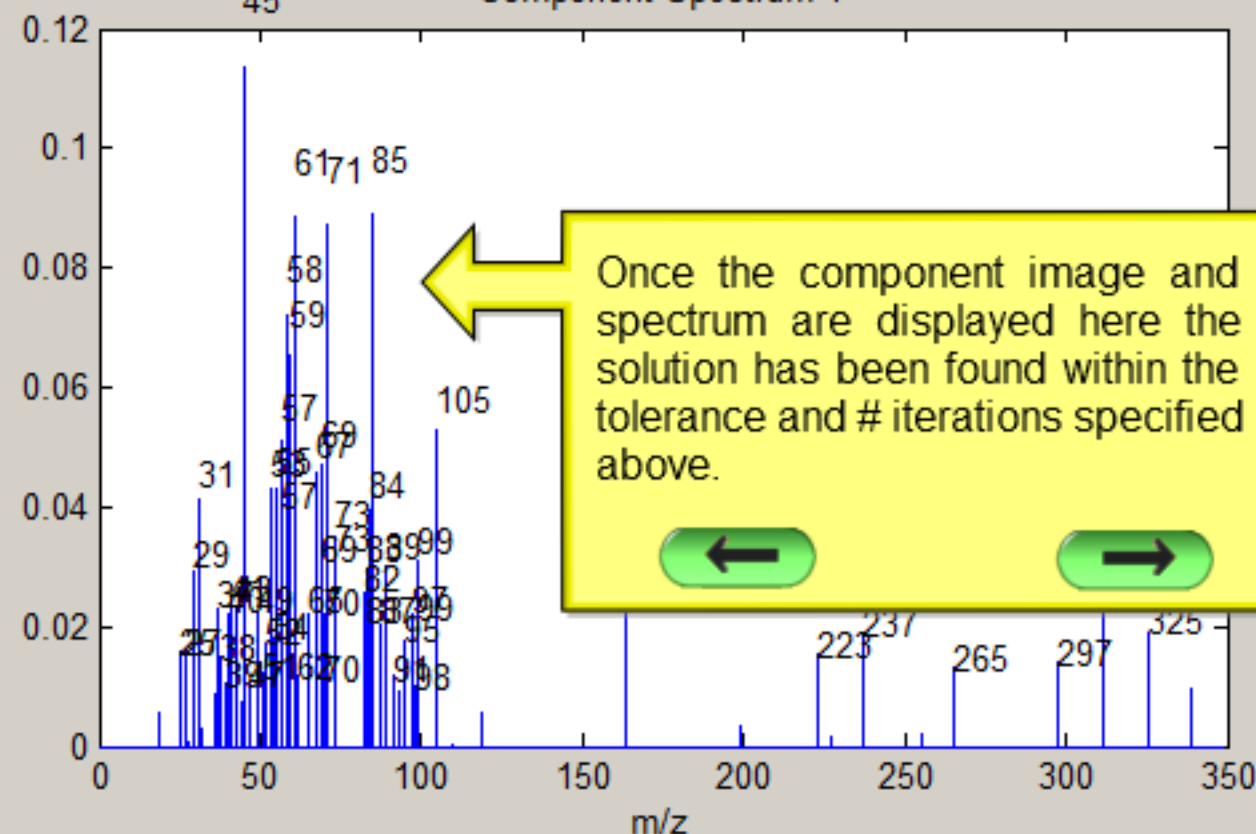
Save Fig

Make Ext

Component Image 1



Component Spectrum 1



Once the component image and spectrum are displayed here the solution has been found within the tolerance and # iterations specified above.

Close panel

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

PoissonScaledM...

exactmass_e2n_1

Scores

Loadings

Variance

PCA_scores ...

Select Loadings

Select Variance

Load Selected Data

Load Selected Scores

inter

10

Tol.

0.1

You must have the MCR-ALS toolbox installed to use this panel

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Depending on
to run MCR. W
first MCR comp

Run MCR

Save MCR Results

Here we can see that component 1 captures the spots. The peaks in the spectrum are indicative of PEG.

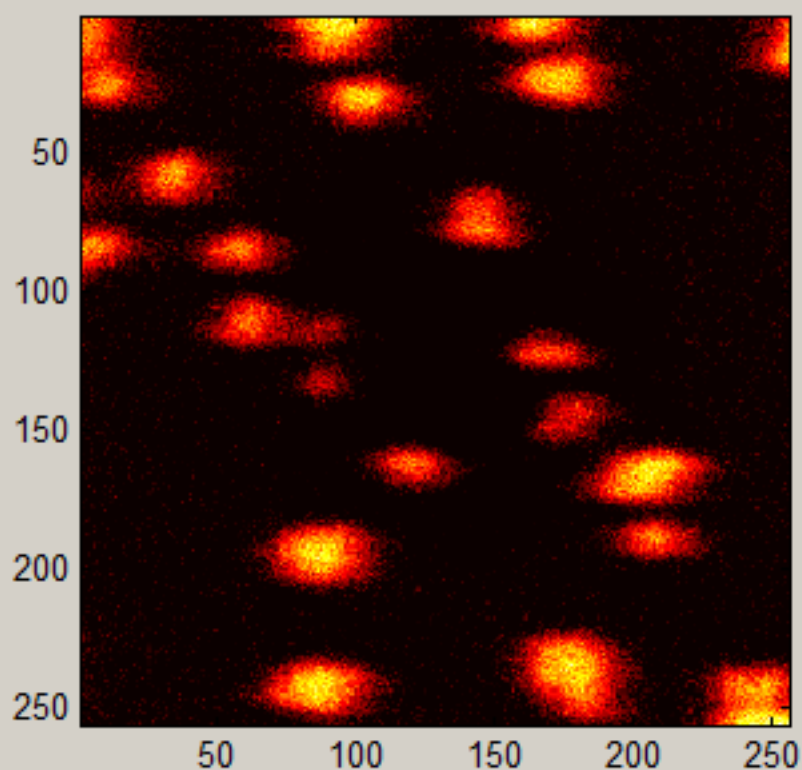
1

All Comp

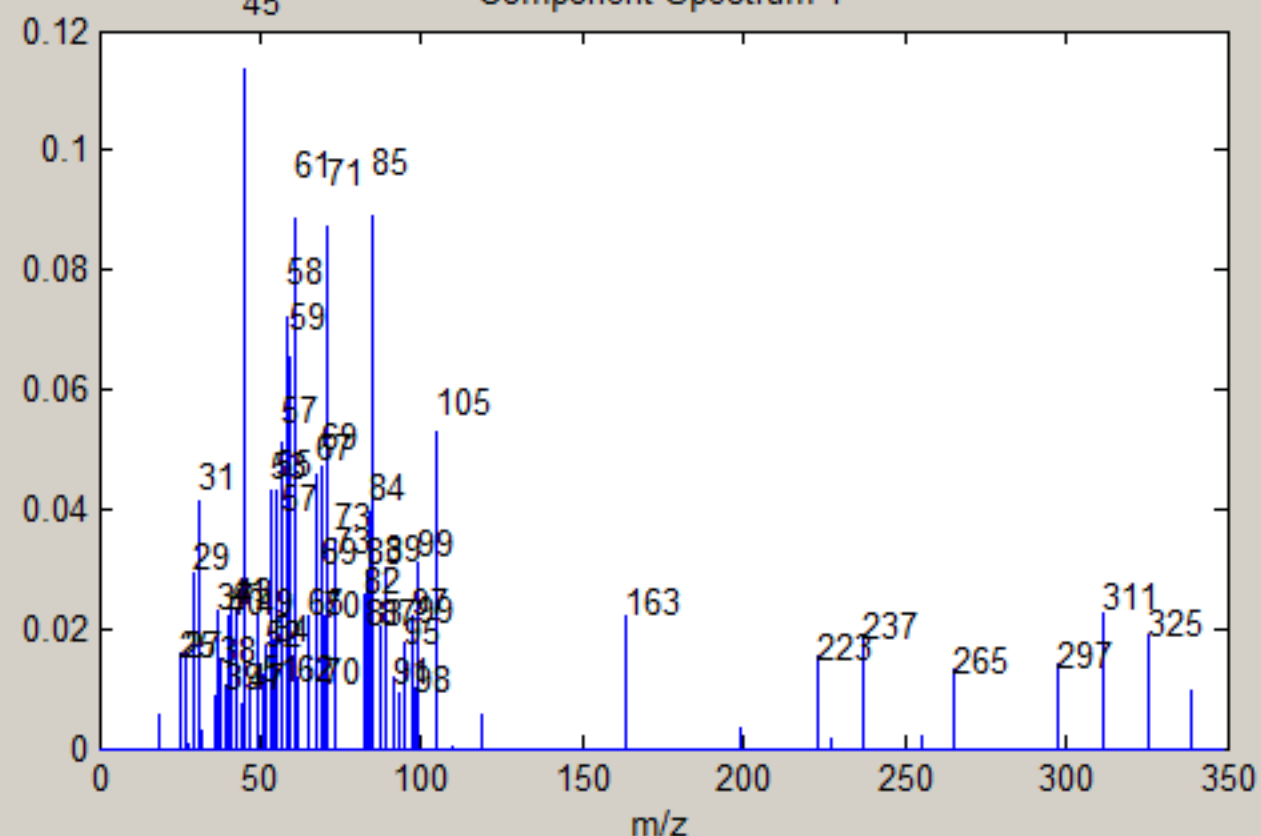
Save Fig

Make Ext

Component Image 1



Component Spectrum 1



Close panel

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

Poisson ScaledM...

exactmass e2n 1

Scores

Loadings

Variance

PCA scores ...

Select Loadings

Select Variance

Load Selected Data

Load Selected Scores

```
# inter
```

10

Tol.

0.1

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Run MCR

Save MCR Results

1

Plot Sel Comp

Plot All Comp

Save Fig

Make Ext

Choose component #

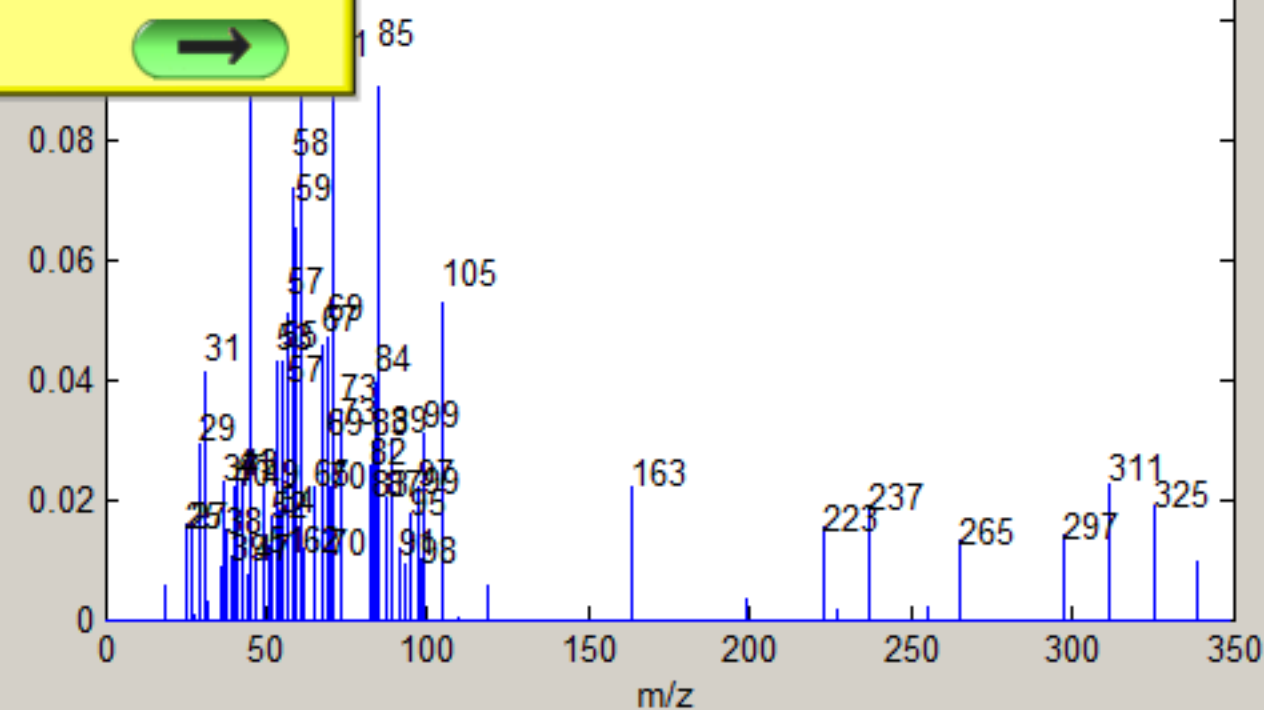
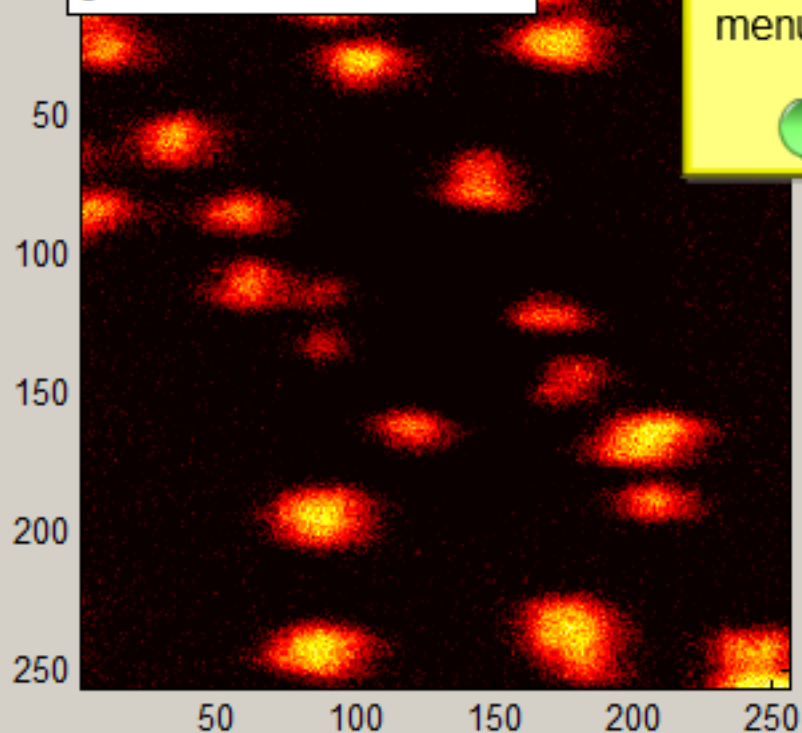
1

2

3

To look at a different component, choose it from this drop down menu.

Component Spectrum 1



Close panel

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

PoissonScaledM...

exactmass_e2n_1

Scores

Loadings

Variance

PCA_scores ...

Select Loadings

Select Variance

Load Selected Data

Load Selected Scores

inter

10

Tol.

0.1

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Run MCR

Save MCR Results

Visit MCR-ALS Website

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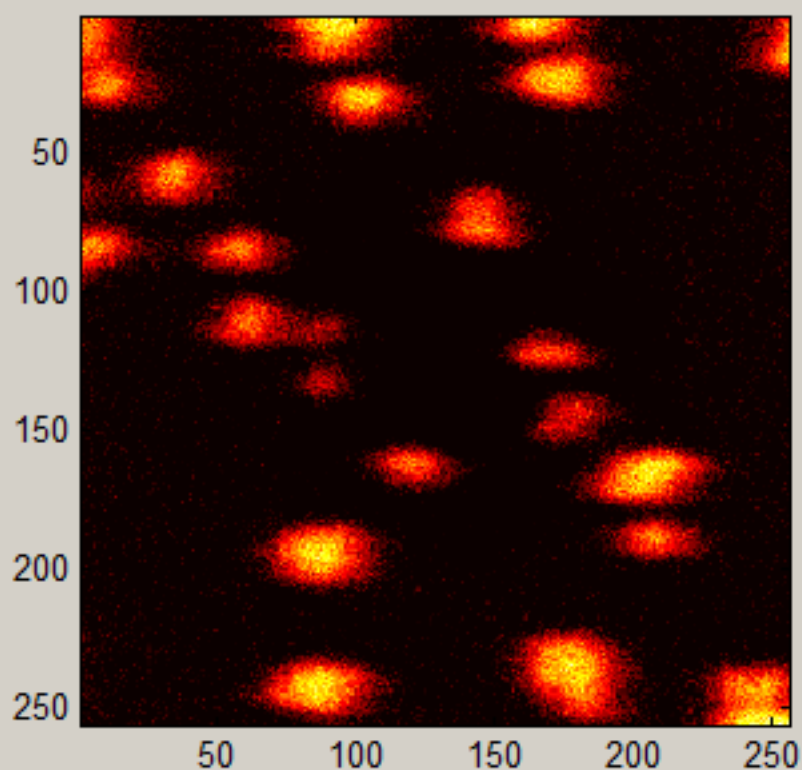
Depending on your data set it can take some time to run MCR. WAIT until you see a plot of the first MCR component to proceed.

2

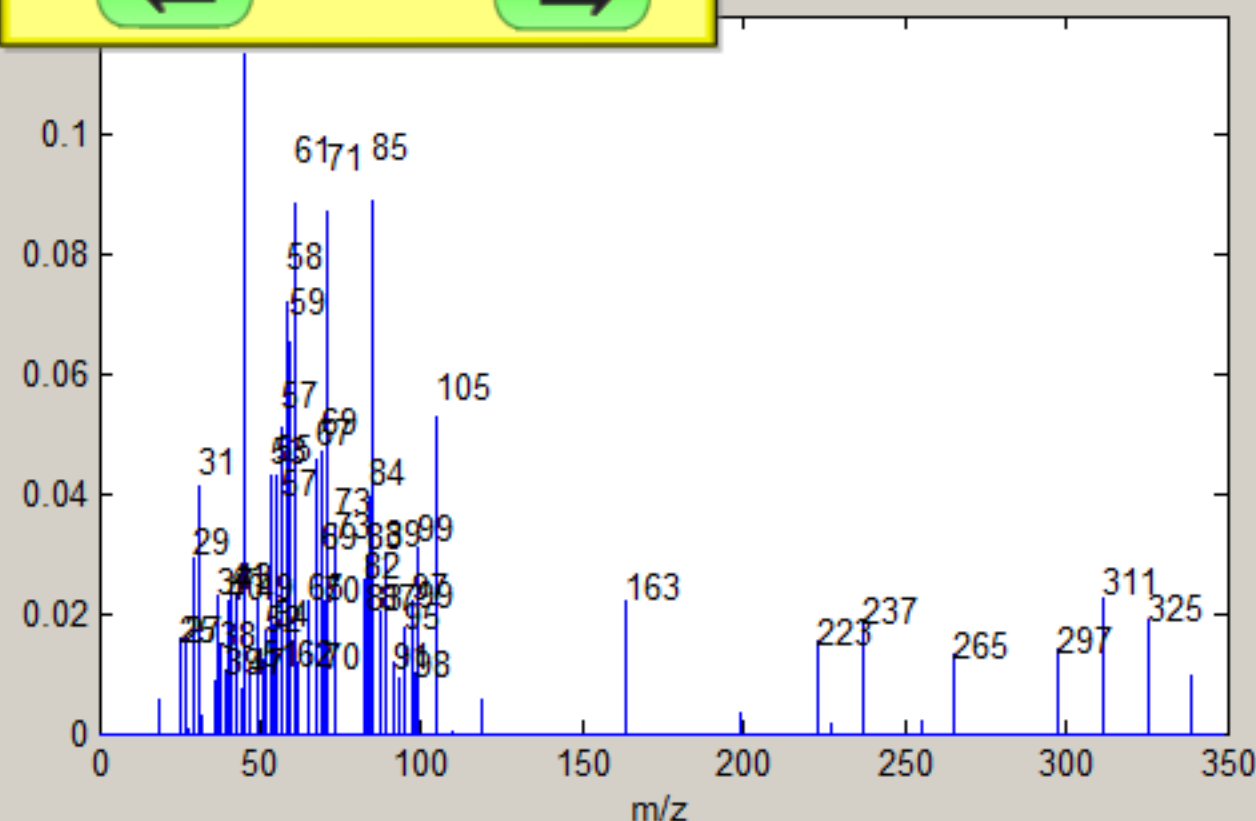
Plot Sel Comp

And press the 'Plot Sel Comp' button.

Component Image 1



Spectrum 1



Close panel

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

PoissonScaledM...

exactmass_e2n_1

Scores

Loadings

Variance

PCA_scores ...

Select Loadings

Select Variance

Load Selected Data

Load Selected Scores

inter

10

Tol.

0.1

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Depending on y
to run MCR. WA
first MCR compo

This component captures the background
and the peaks are indicative of the silane
linker used on this sample.

Let's select component 3.

Run MCR

Save MCR Results

All Comp

Save Fig

Make Ext

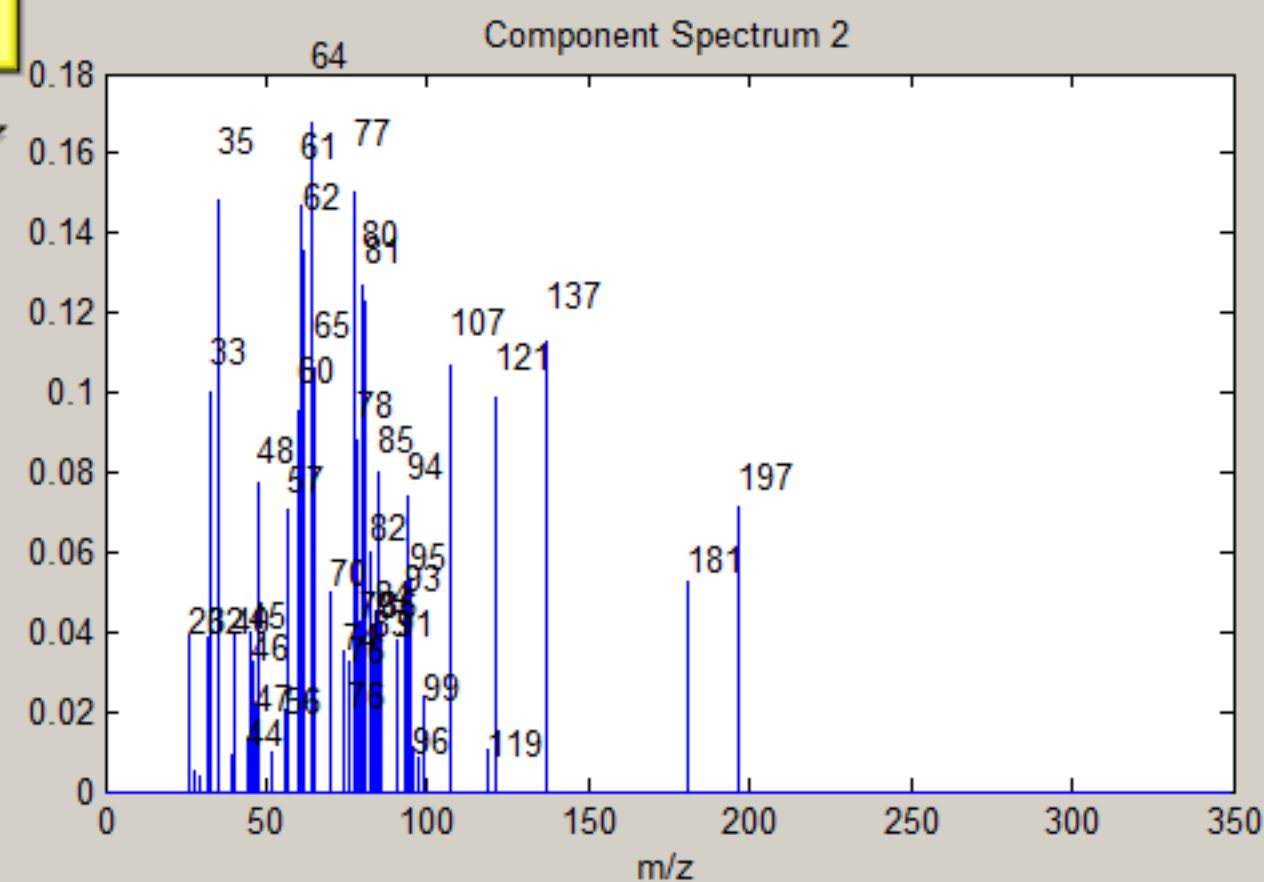
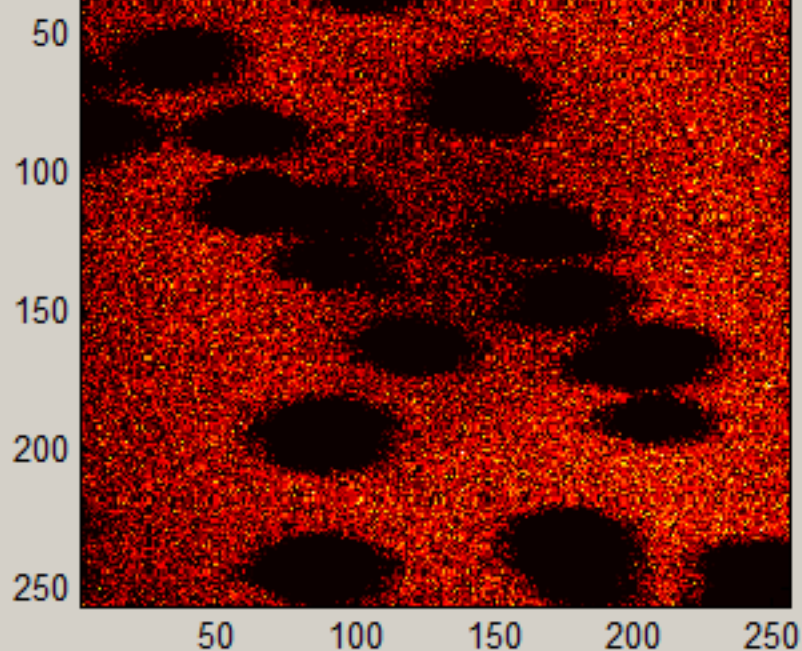
2

Choose

1

2

3



Close panel

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

Poisson ScaledM...

exactmass e2n 1

Scores

Loadings

Variance

PCA scores ...

Select Loadings

Select Variance

Load Selected Data

Load Selected Scores

Image: PoissonScaledMC
Variables: exactmass e2n 1

or use:

Init Est: PCA scores

```
# inter
```

10

Tol.

0.1

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Run MCR

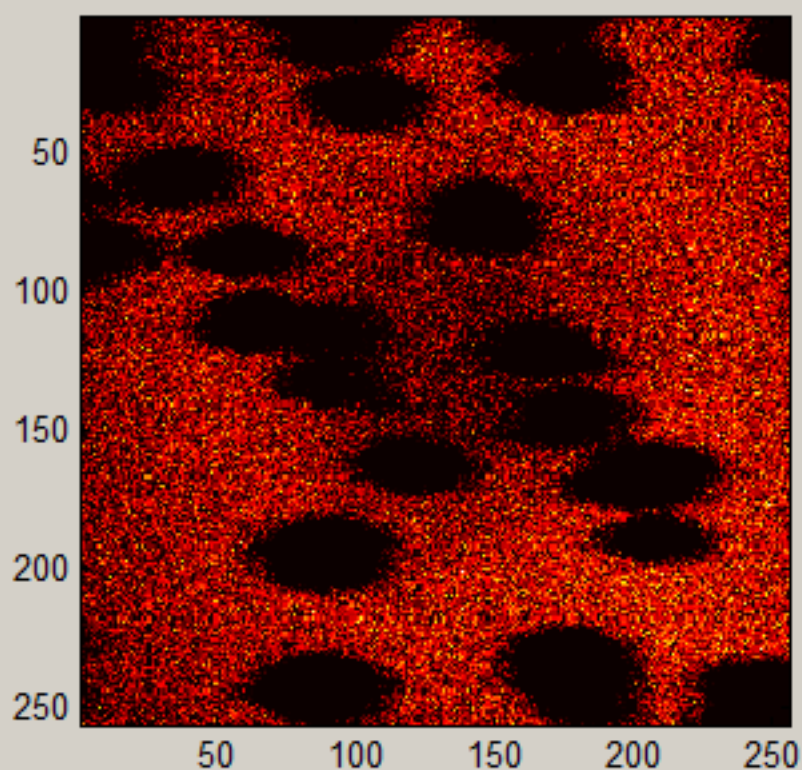
Save MCR Results

2

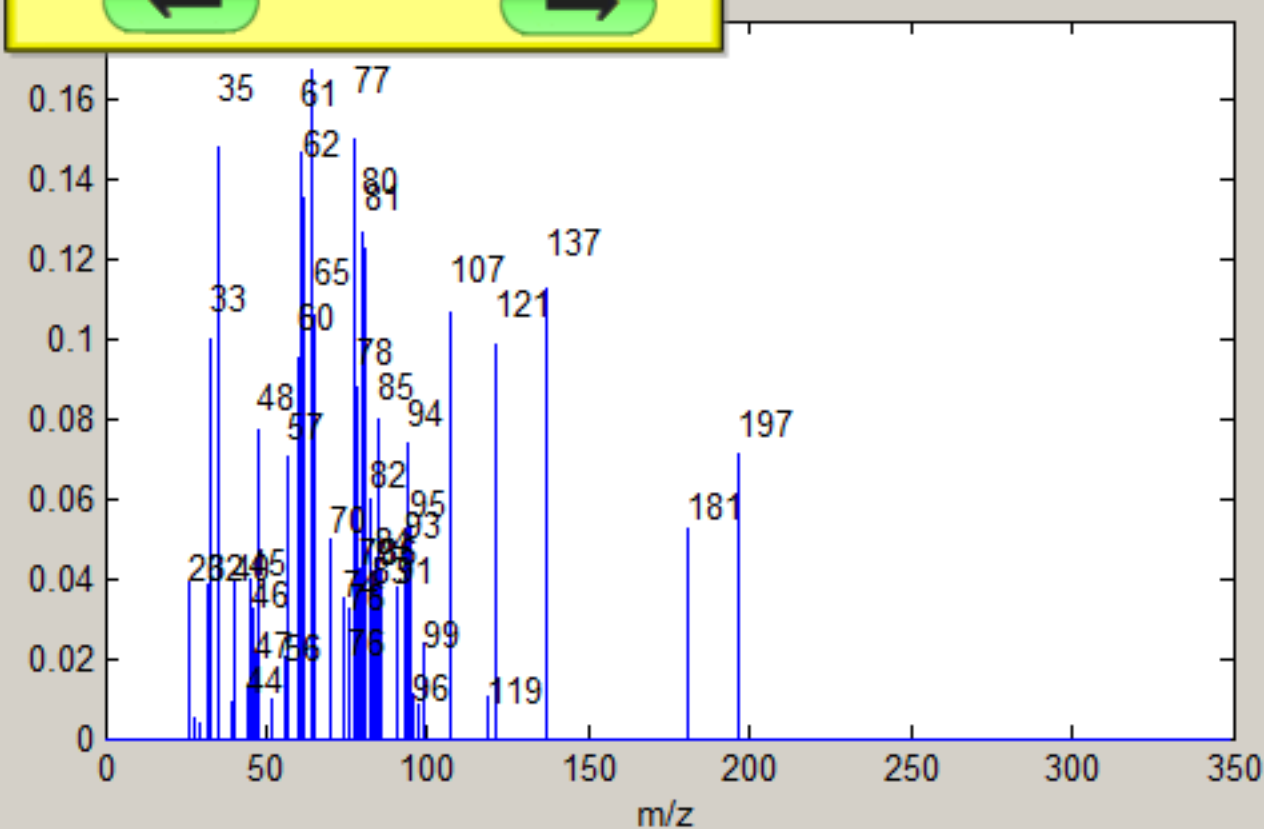
Plot Sel Comp

And press the 'Plot Sel Comp' button.

Component Image 2



Spectrum 2



Close panel

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

PoissonScaledM...

exactmass_e2n_1

Scores

Loadings

Variance

PCA_scores ...

Select Loadings

Select Variance

Load Selected Data

Load Selected Scores

inter

10

Tol.

0.1

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to run MCR. Wait for the first MCR component

Run MCR

Save MCR Results

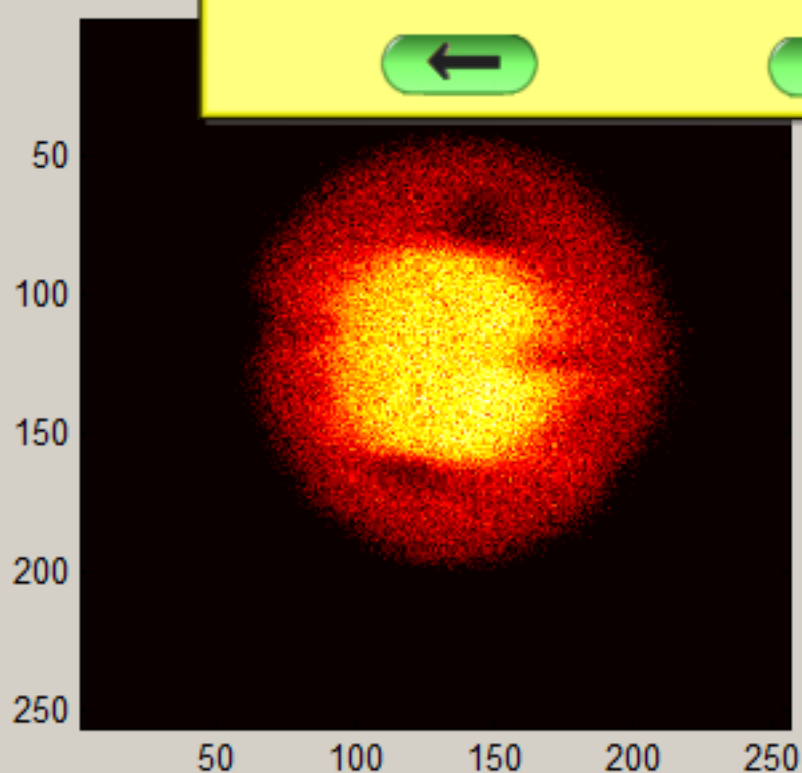
Component 3 shows the DNA spot and the
peaks are fragments typical of DNA.

So it looks like the assumption of 3 components
was logical. However, this may not always be
the case. You typically have to look at several
solutions in order to determine which one makes
the most sense.

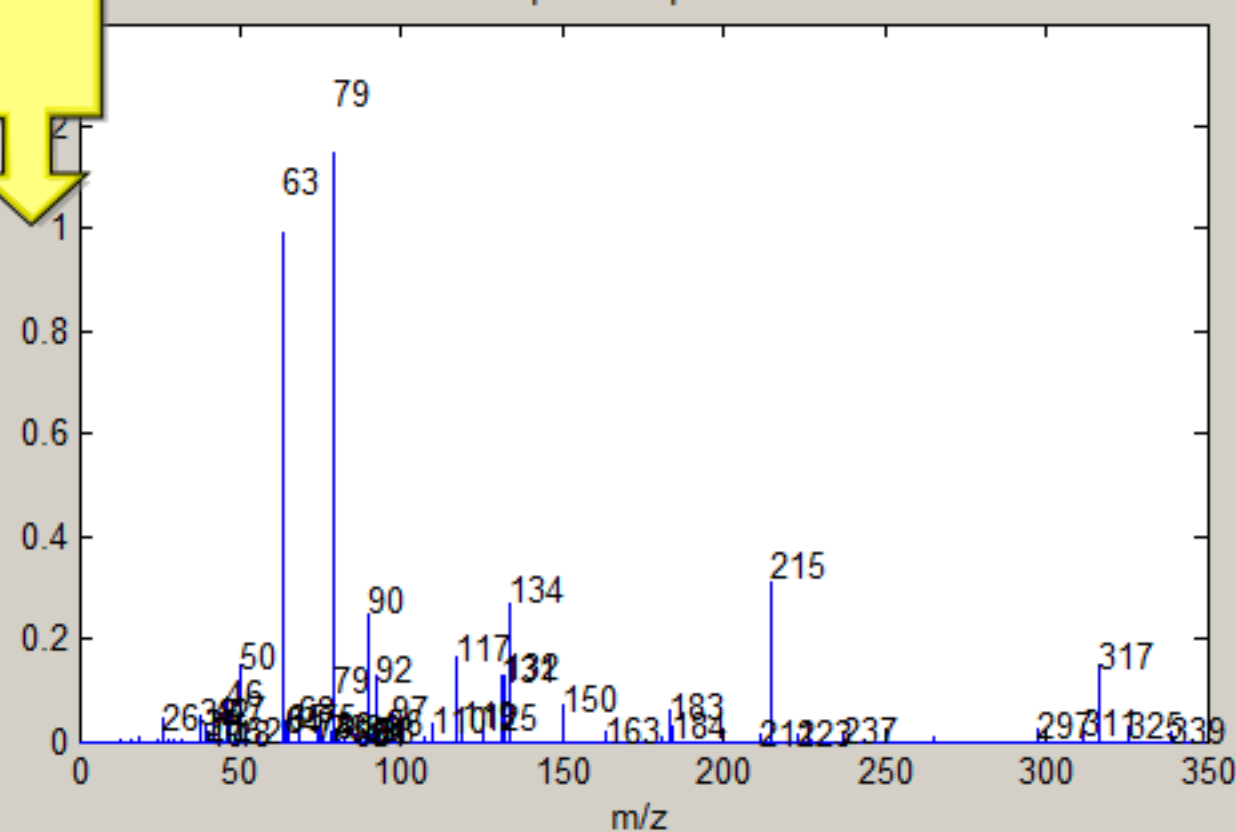
3

Save Fig

Make Ext



Component Spectrum 3



Close panel

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

PoissonScaledM...

exactmass_e2n_1

Scores

Loadings

Variance

PCA_scores ...

Select Loadings

Select Variance

Load Selected Data

Load Selected Scores

inter

10

Tol.

0.1

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Run MCR

Save MCR Results

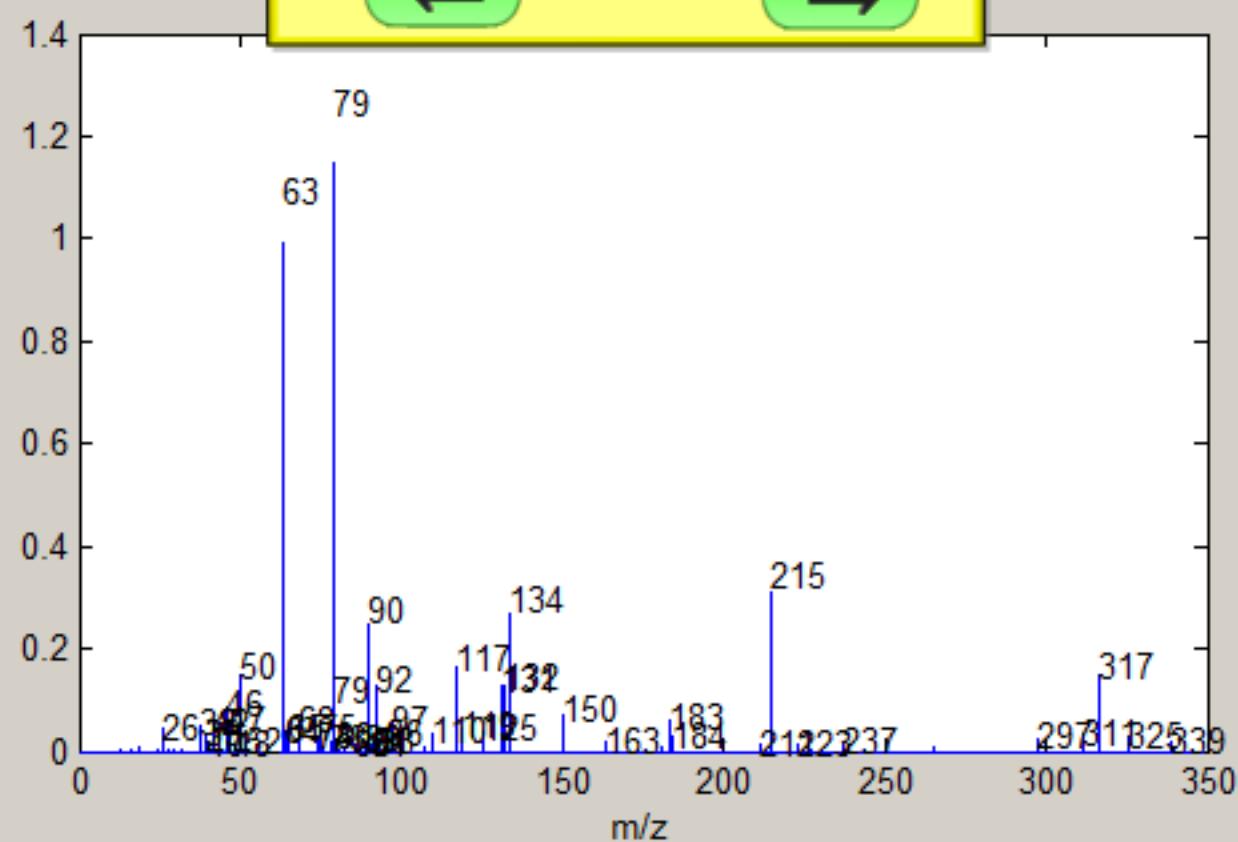
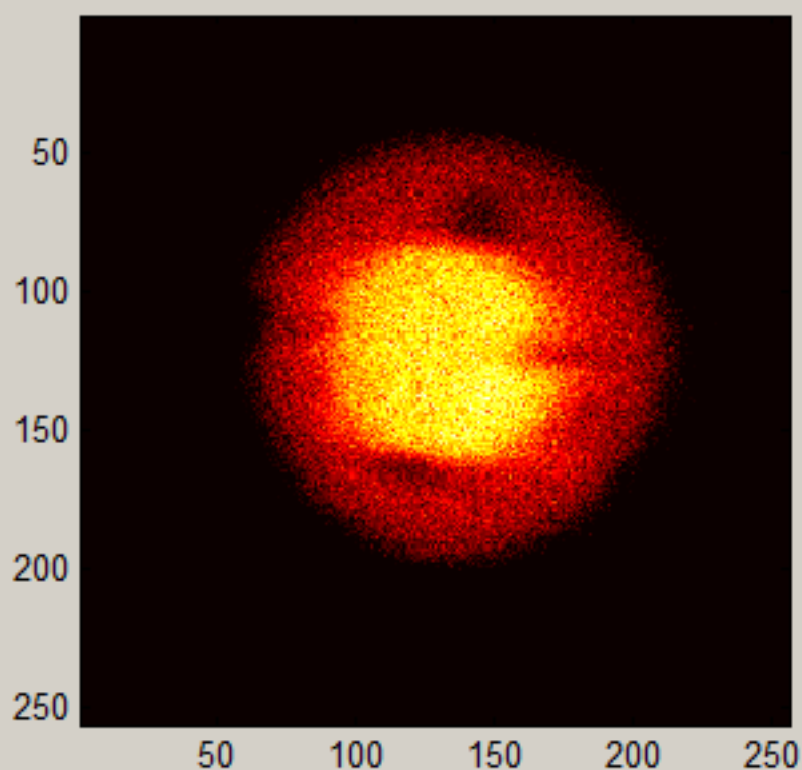
3

Plot Sel Comp

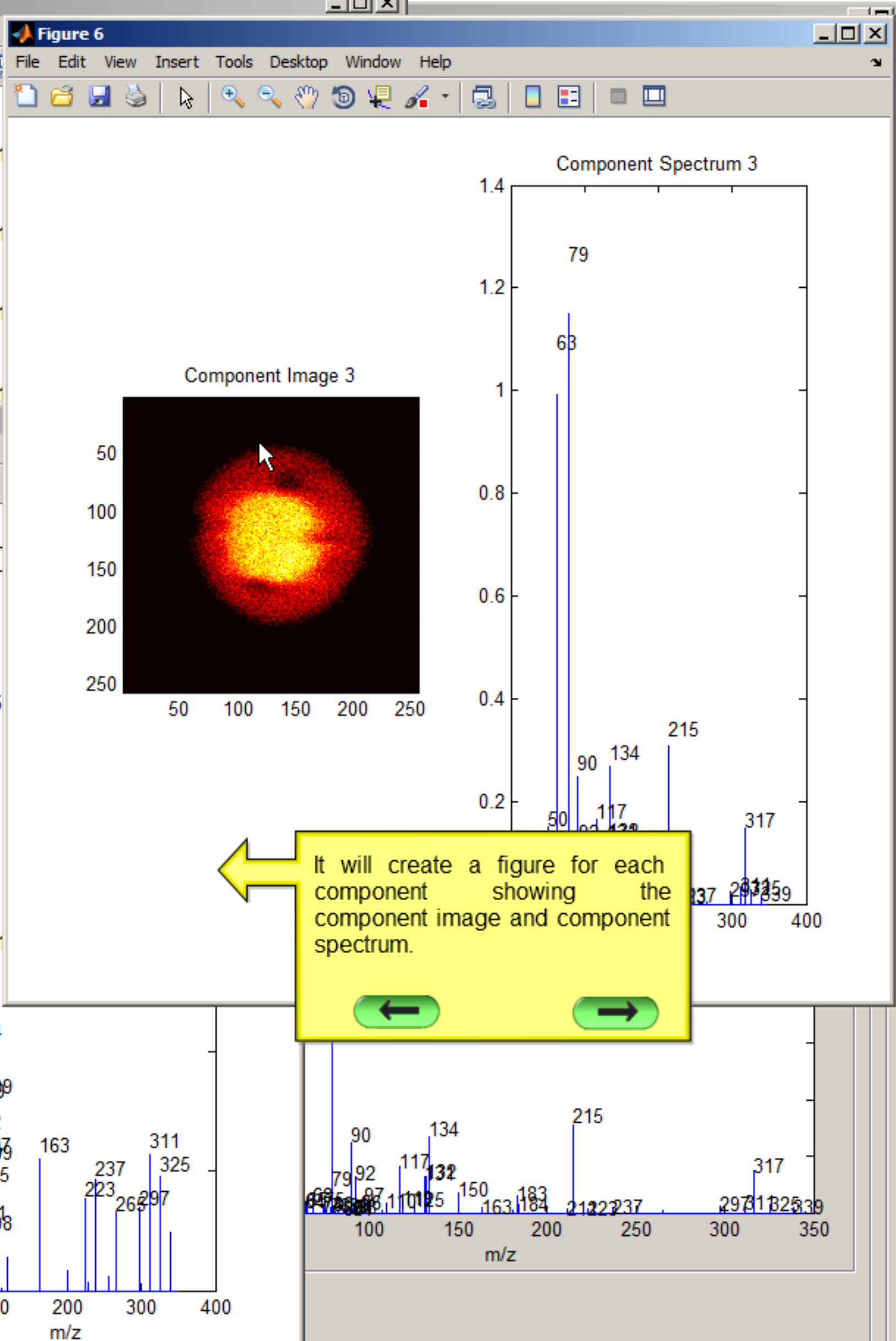
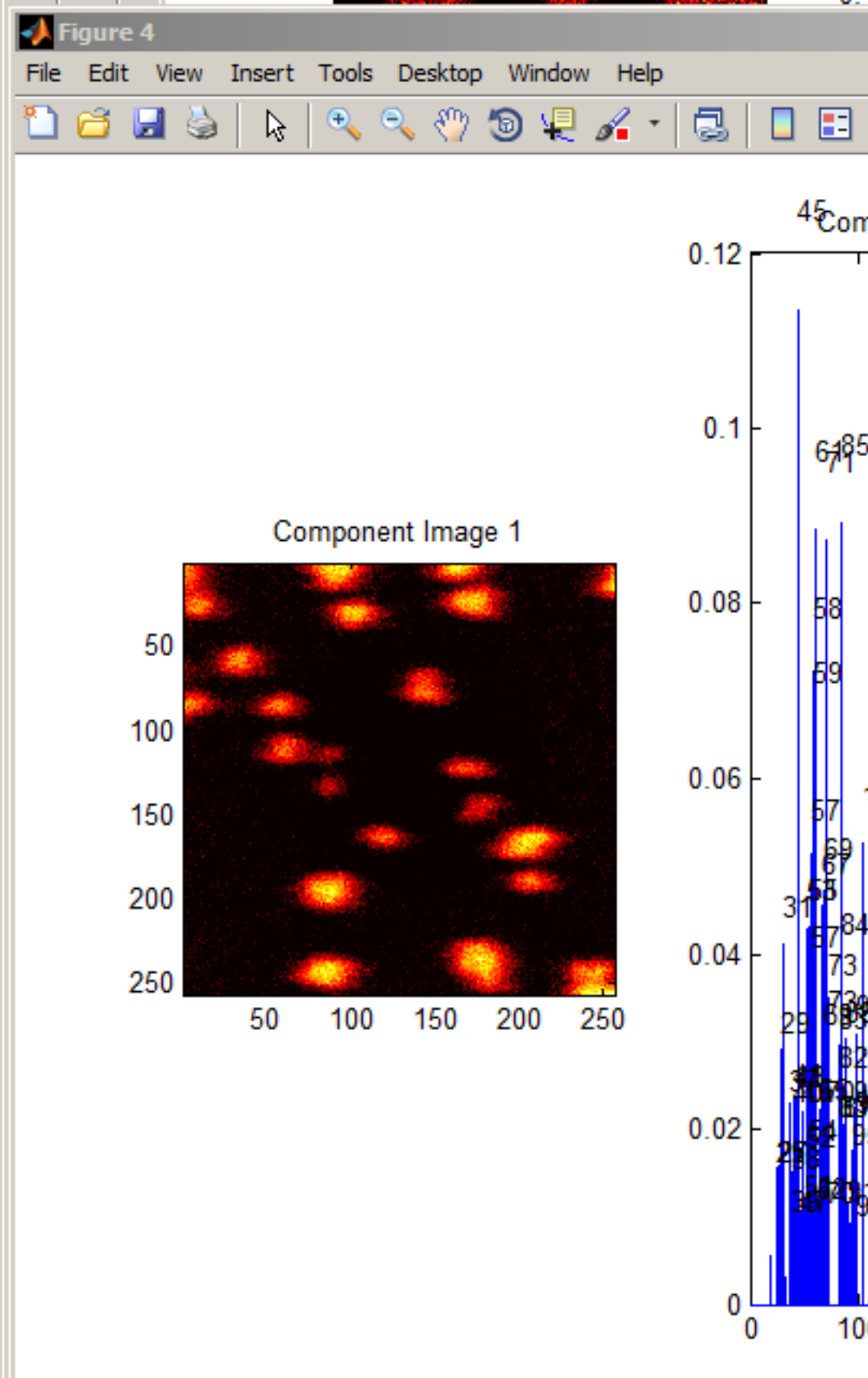
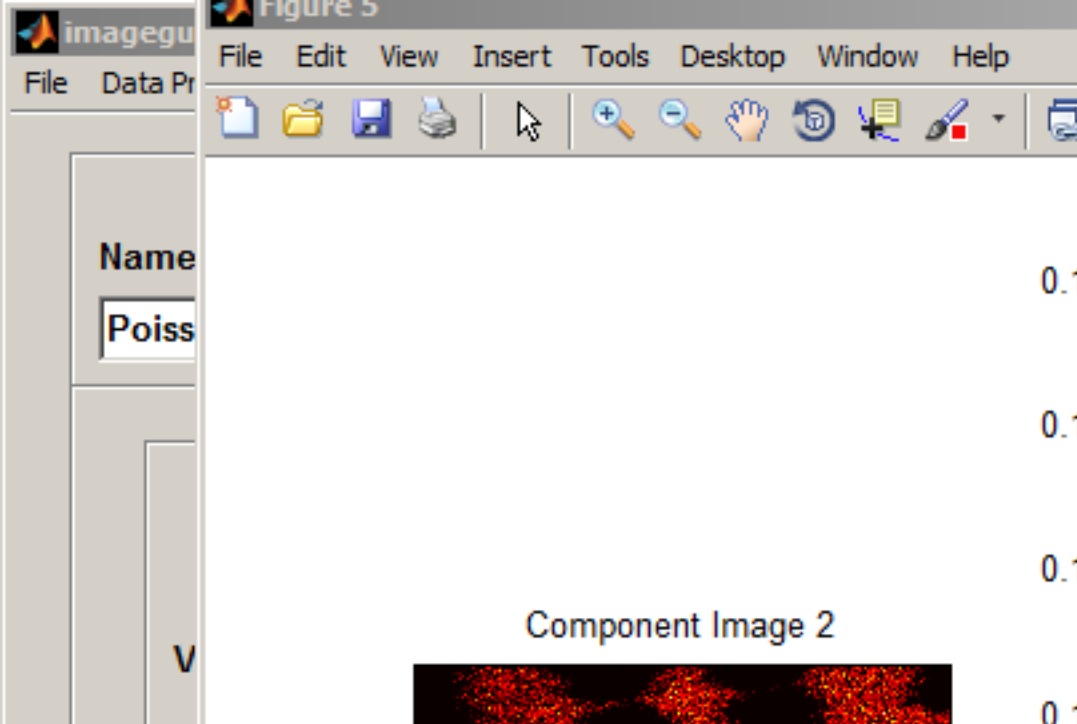
Plot All Comp

If you press the 'Plot All Comp' button...

Component Image 3



Close panel



Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

PoissonScaledM...

exactmass_e2n_1

Scores

Loadings

Variance

PCA_scores ...

Select Loadings

Select Variance

Load Selected Data

Load Selected Scores

inter

10

Tol.

0.1

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Run MCR

Save MCR Results

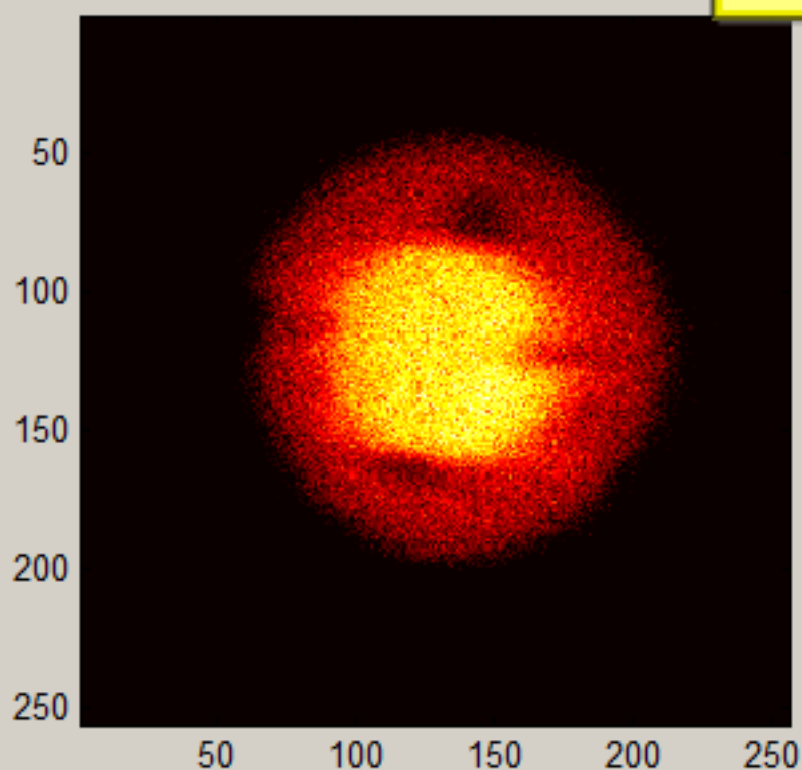
3

Plot

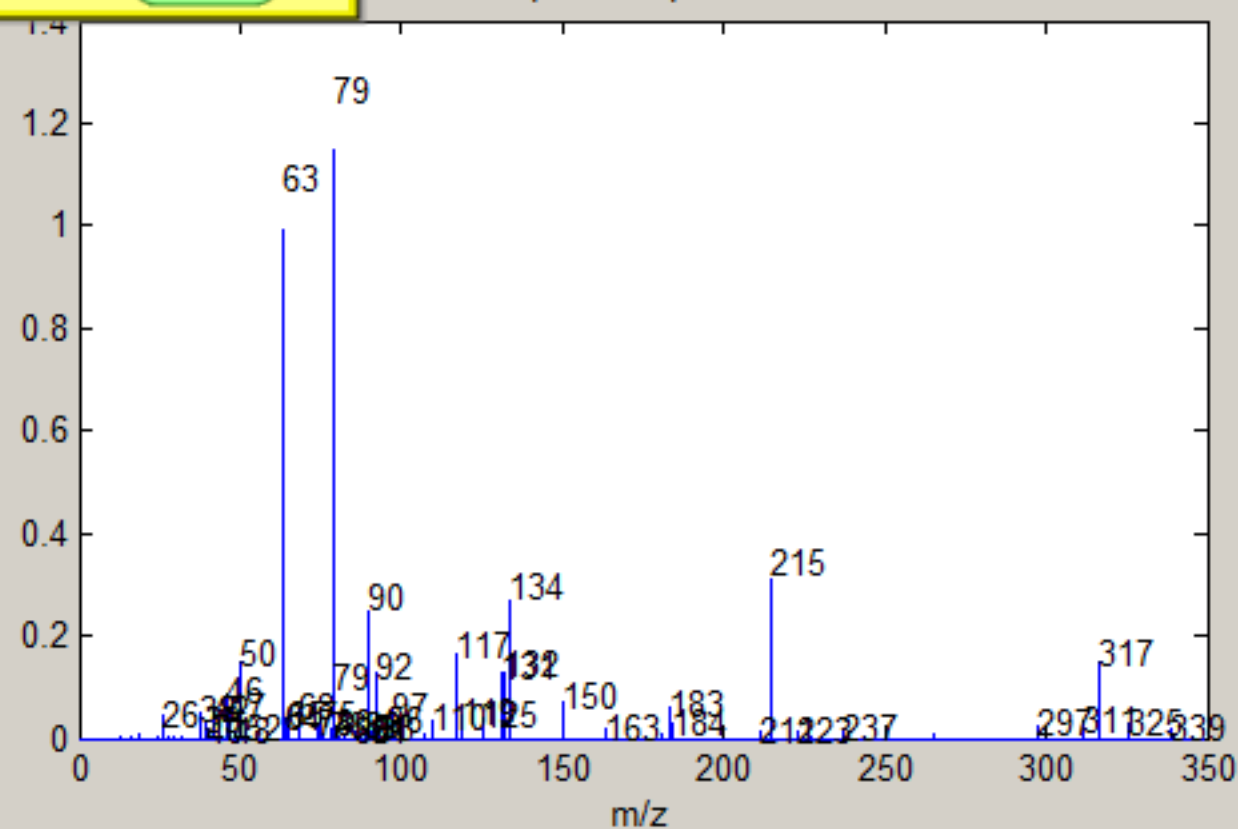
Pressing the 'Make Ext' button...

Make Ext

Component Image 3



Component Spectrum 3



Close panel

Data

Name of Image Matrix

Name of Variable Matrix

PoissonScaledM...

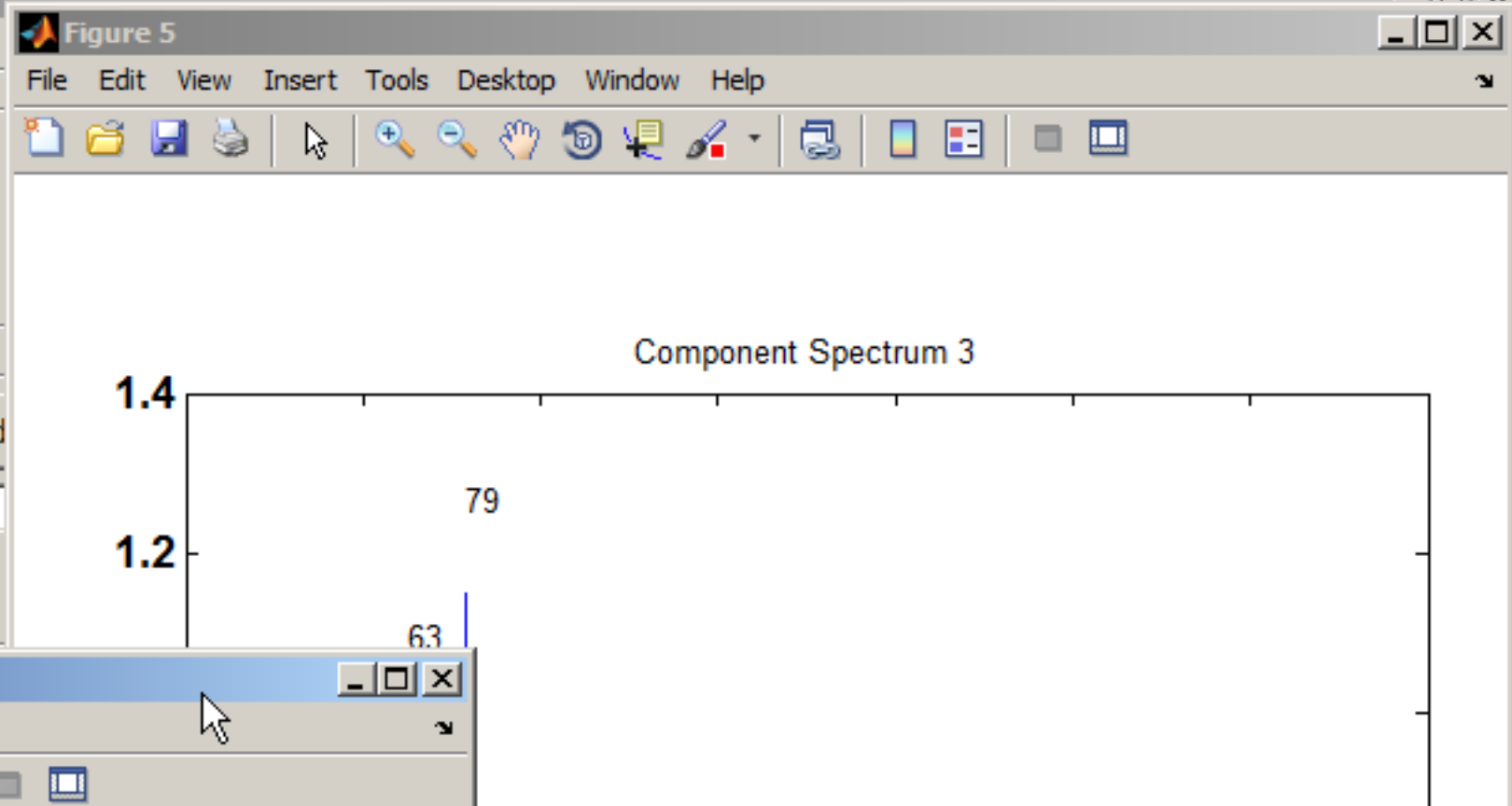
exactmass_e2n_1

Load Selected Data

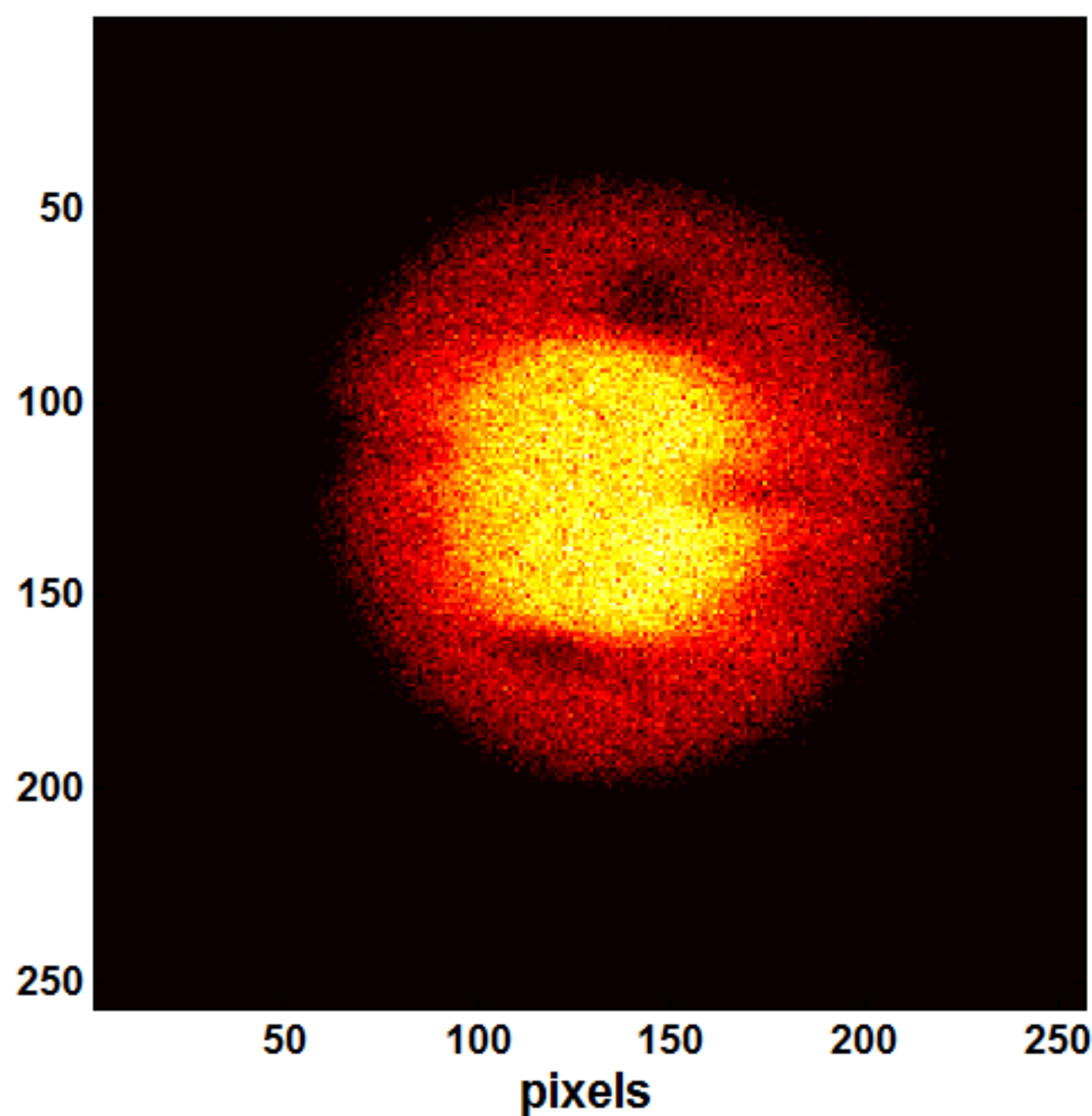
Load

Image: PoissonScaledMC
Variables: exactmass_e2n_1

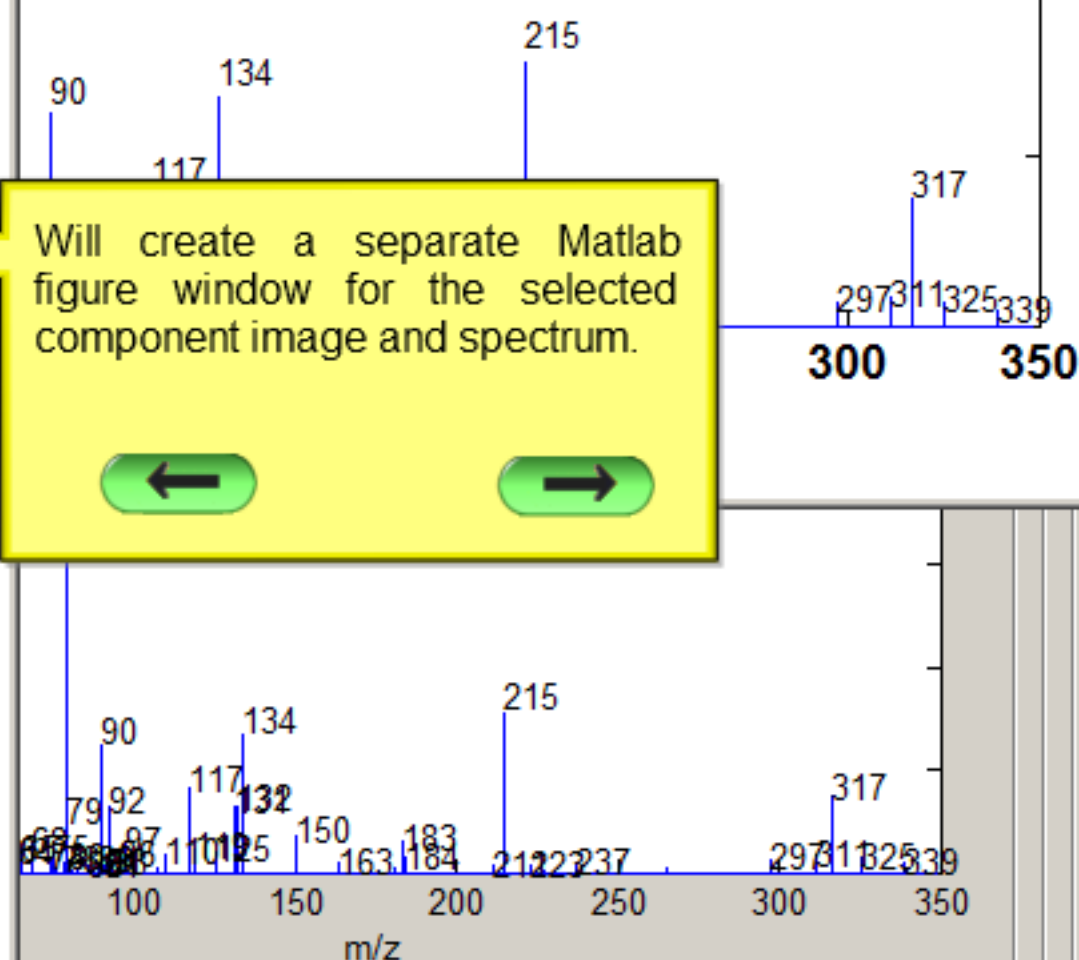
or use:
Init Est:



Component Image 3



Will create a separate Matlab figure window for the selected component image and spectrum.



Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

PoissonScaledM...

exactmass_e2n_1

Scores

Loadings

Variance

PCA_scores ...

Select Loadings

Select Variance

Load Selected Data

Load Selected Scores

inter

10

Tol.

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Run MCR

Save MCR Results

3

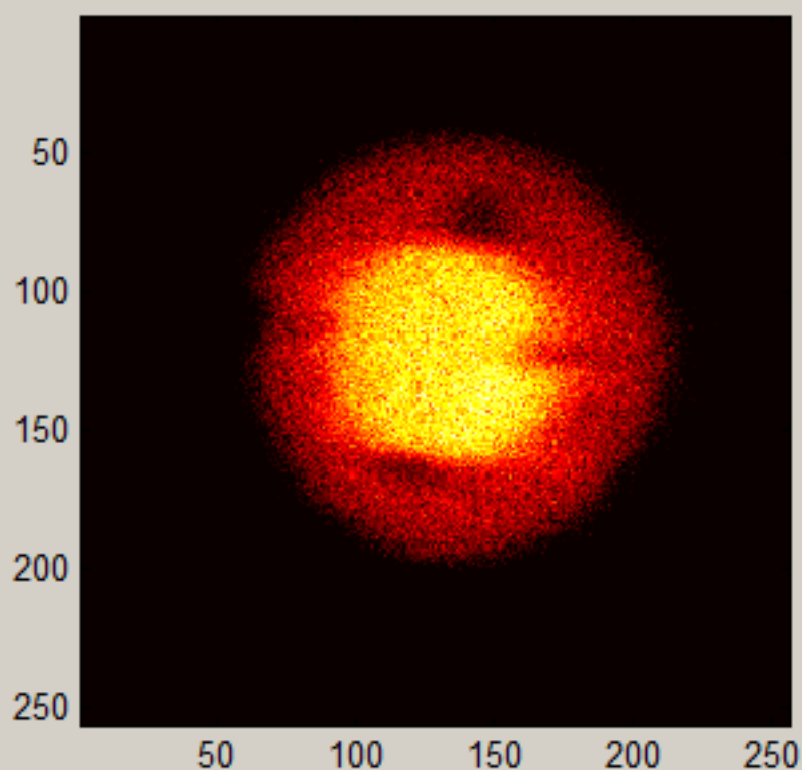
Plot Sel Comp

Plot All Comp

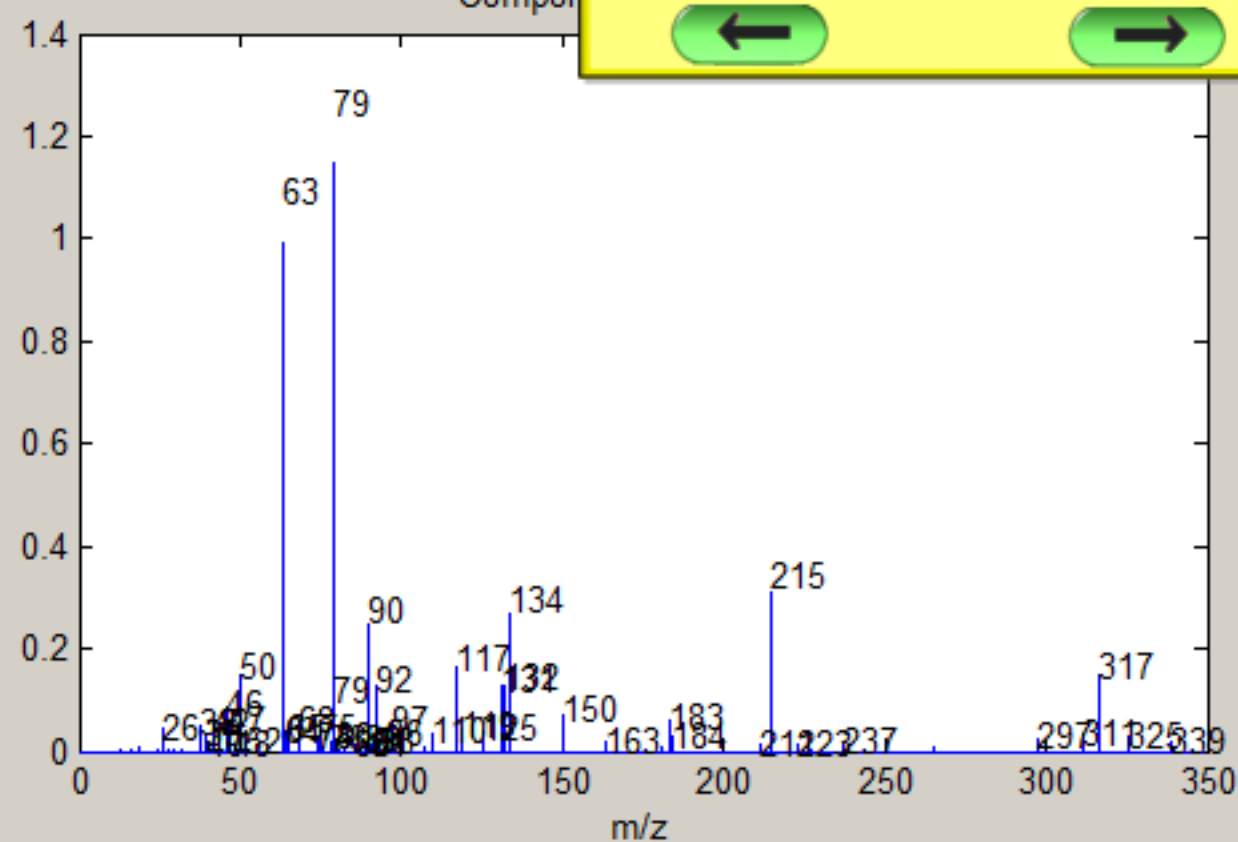
Save Fig

Pressing the 'Save Fig' button will open dialogs so you can save the component image and spectrum for the selected component.

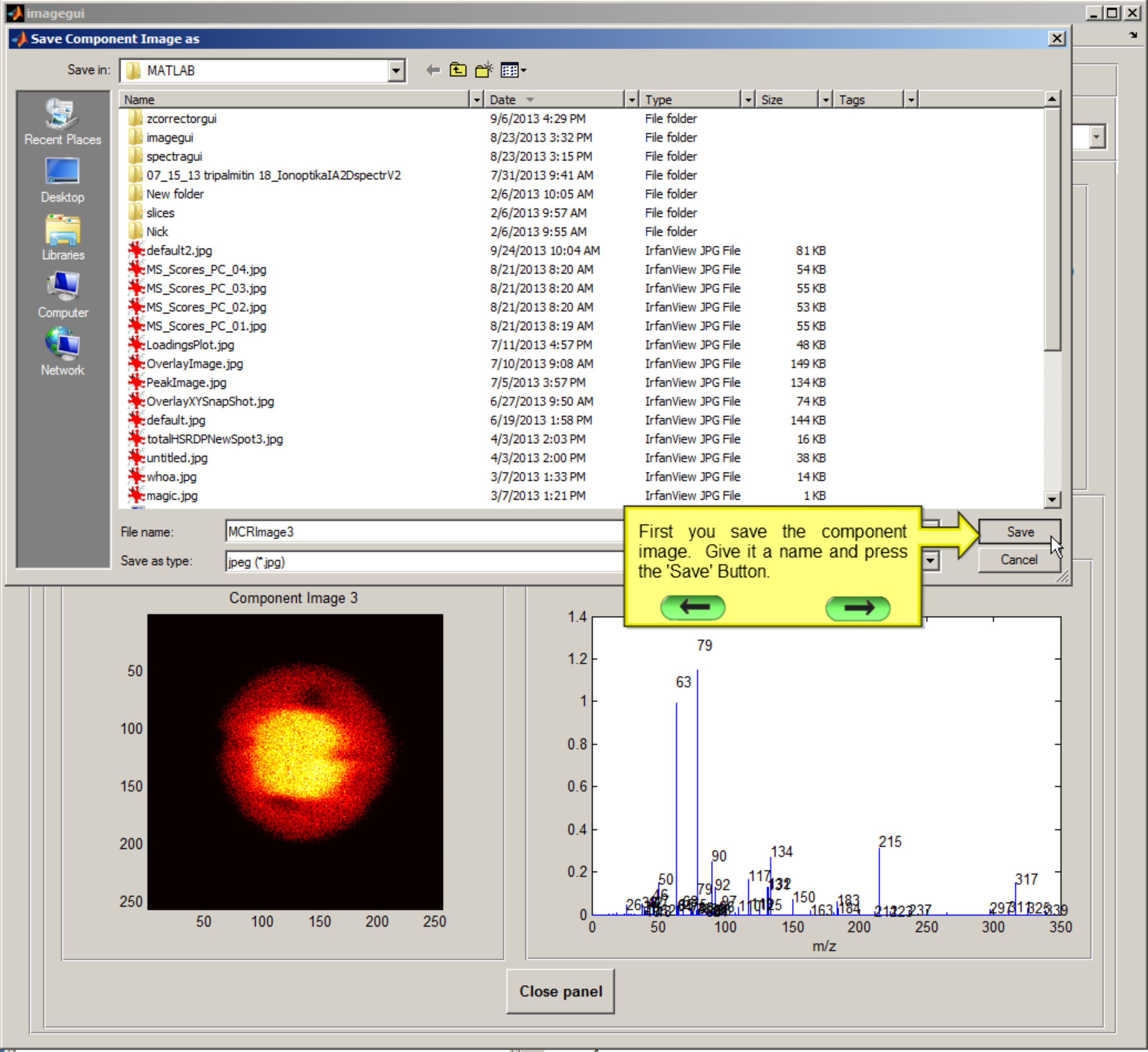
Component Image 3

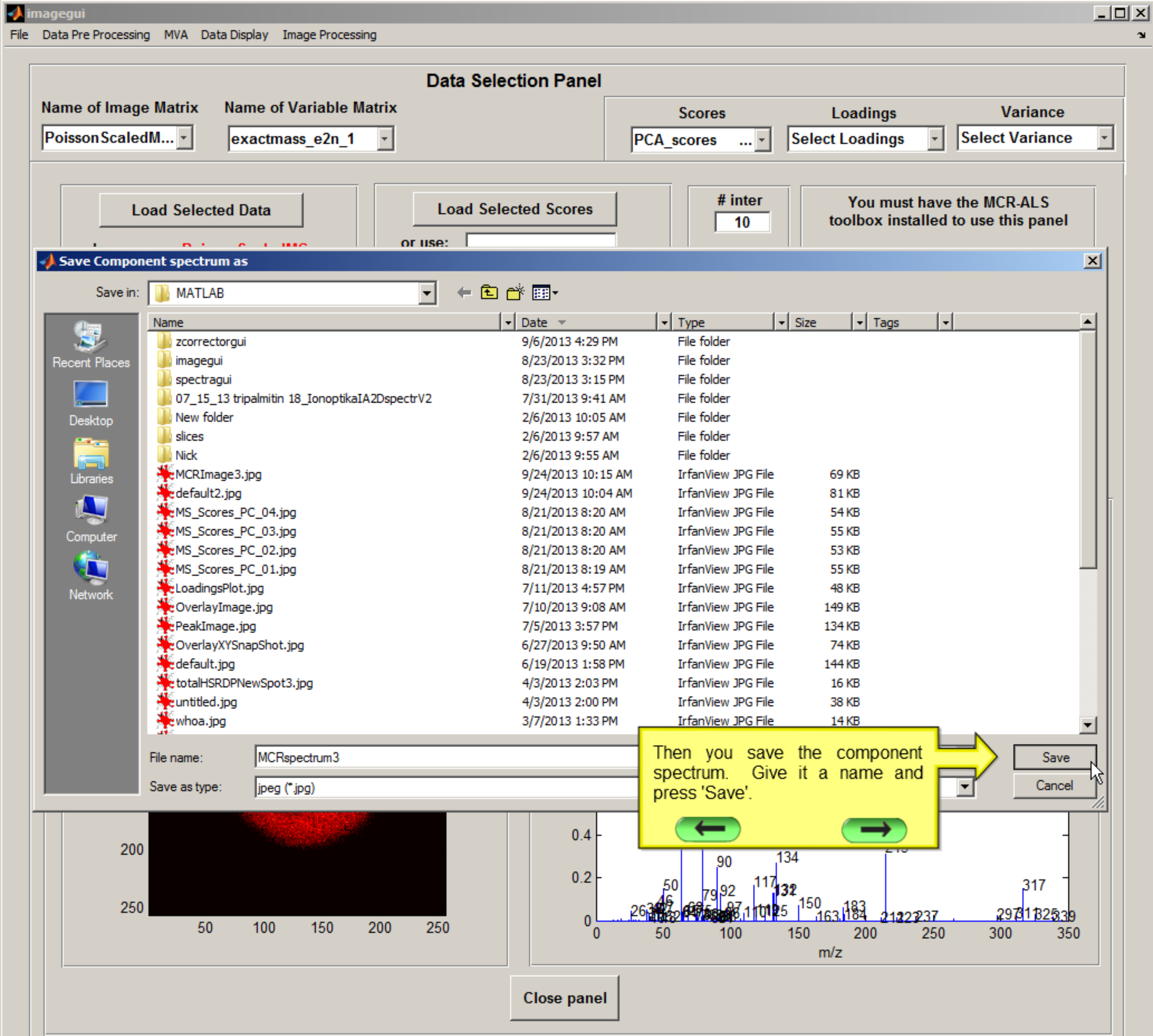


Component Spectrum



Close panel





imagegui

File Data Pre Processing MVA Data Display Image Processing

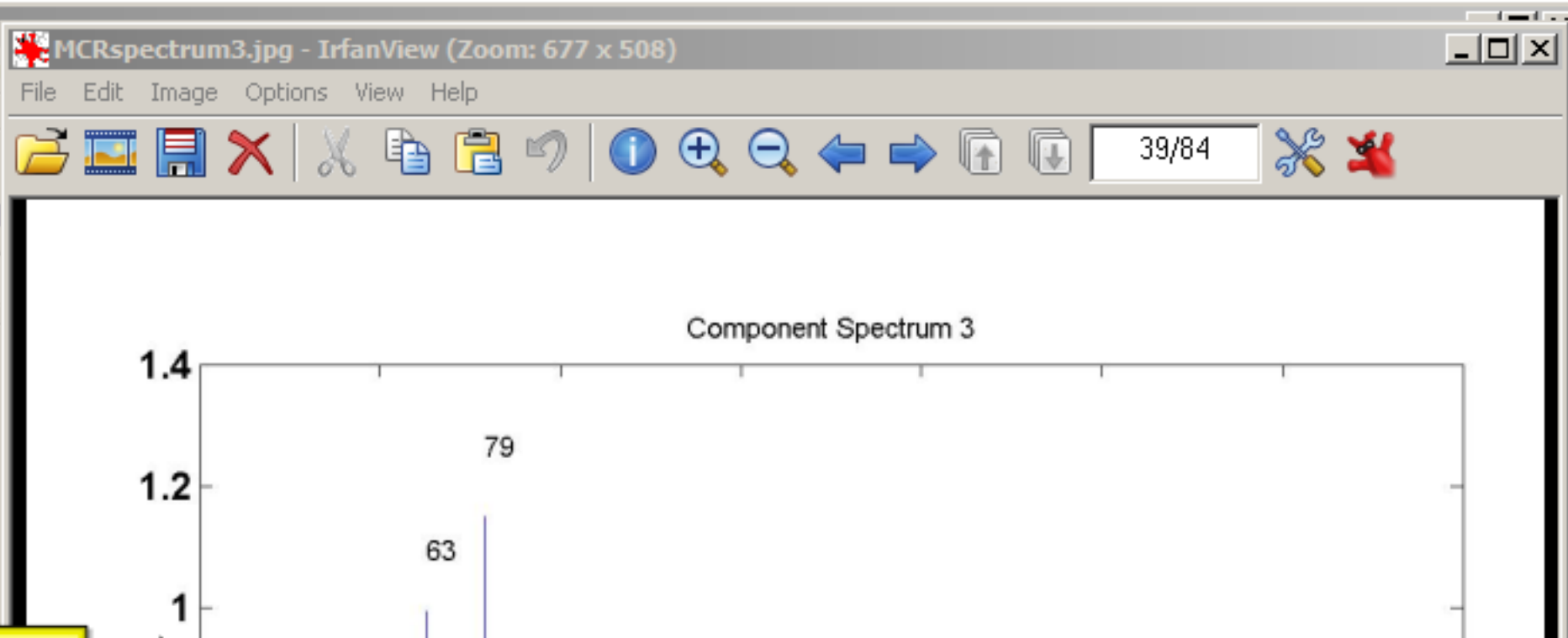
Name of Image Matrix: PoissonScaledM...

Name of Variable Matrix: exactmass_e2n_1

Load Selected Data

Image: PoissonScaledMC

Variables: exactmass_e2n_1

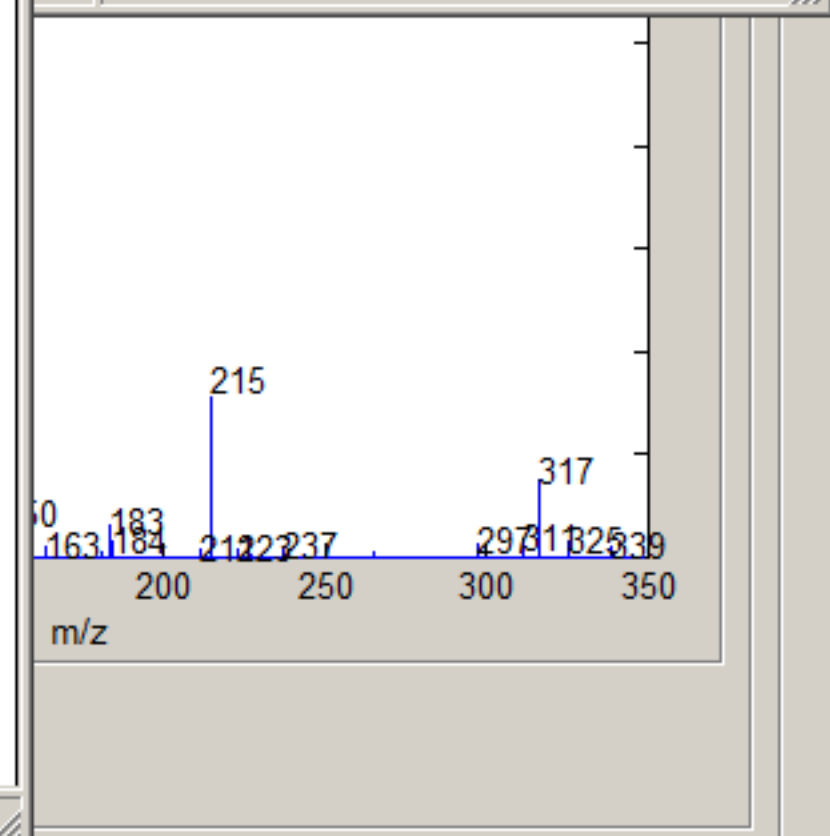
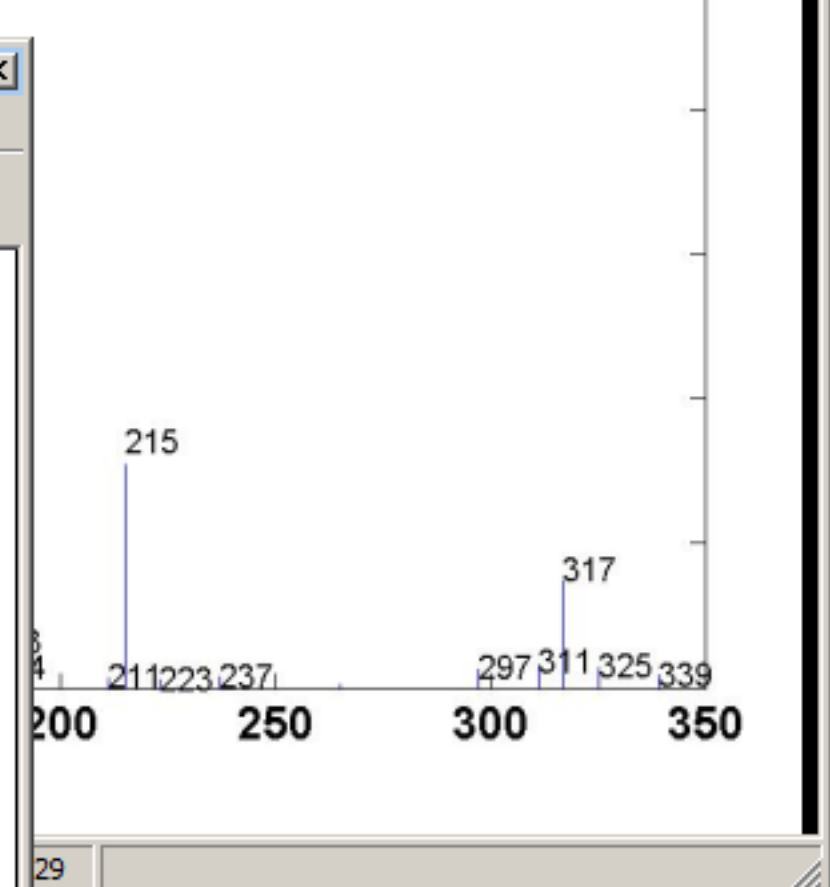
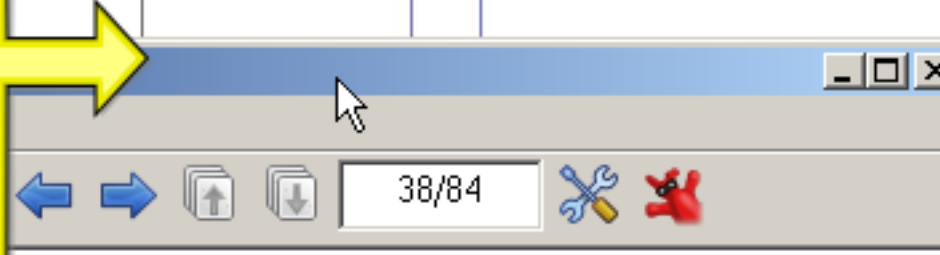


MCRImage3

File Edit Image

Here I have opened the saved images to show they were saved properly.

← →



Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

PoissonScaledM...

exactmass_e2n_1

Scores

Loadings

Variance

PCA_scores ...

Select Loadings

Select Variance

Load Selected Data

Load Selected Scores

inter

10

Tol.

0.1

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Depending on y
to run MCR. WA
first MCR compo

Press the 'Save MCR Results' to export the component image and spectrum data into tab delimited text files. The files contain the data from each component in a separate column. The data can be imported into any program that will accept tab delimited text files.

Run MCR

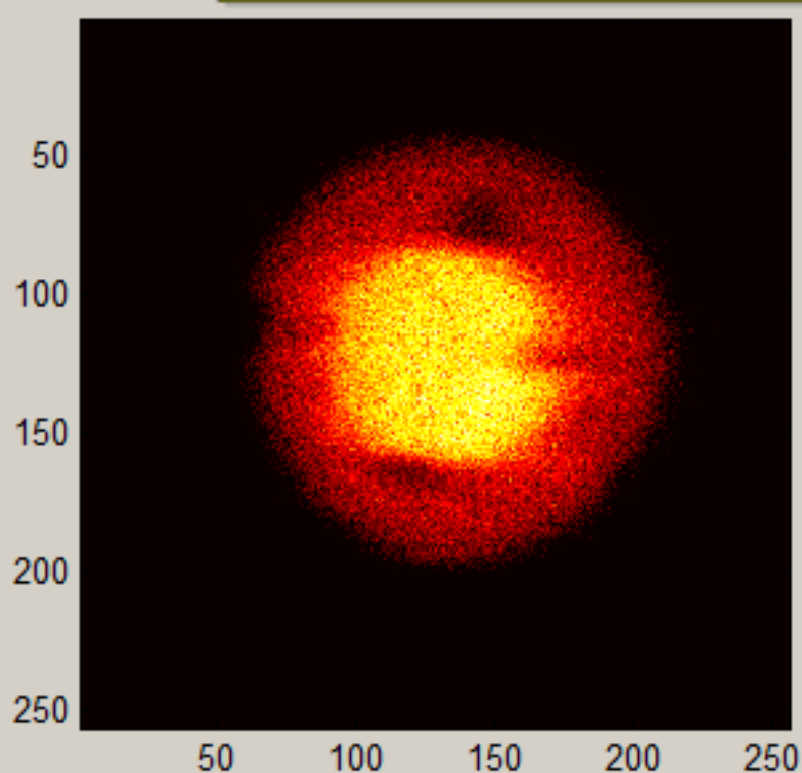
Save MCR Results

Plot All Comp

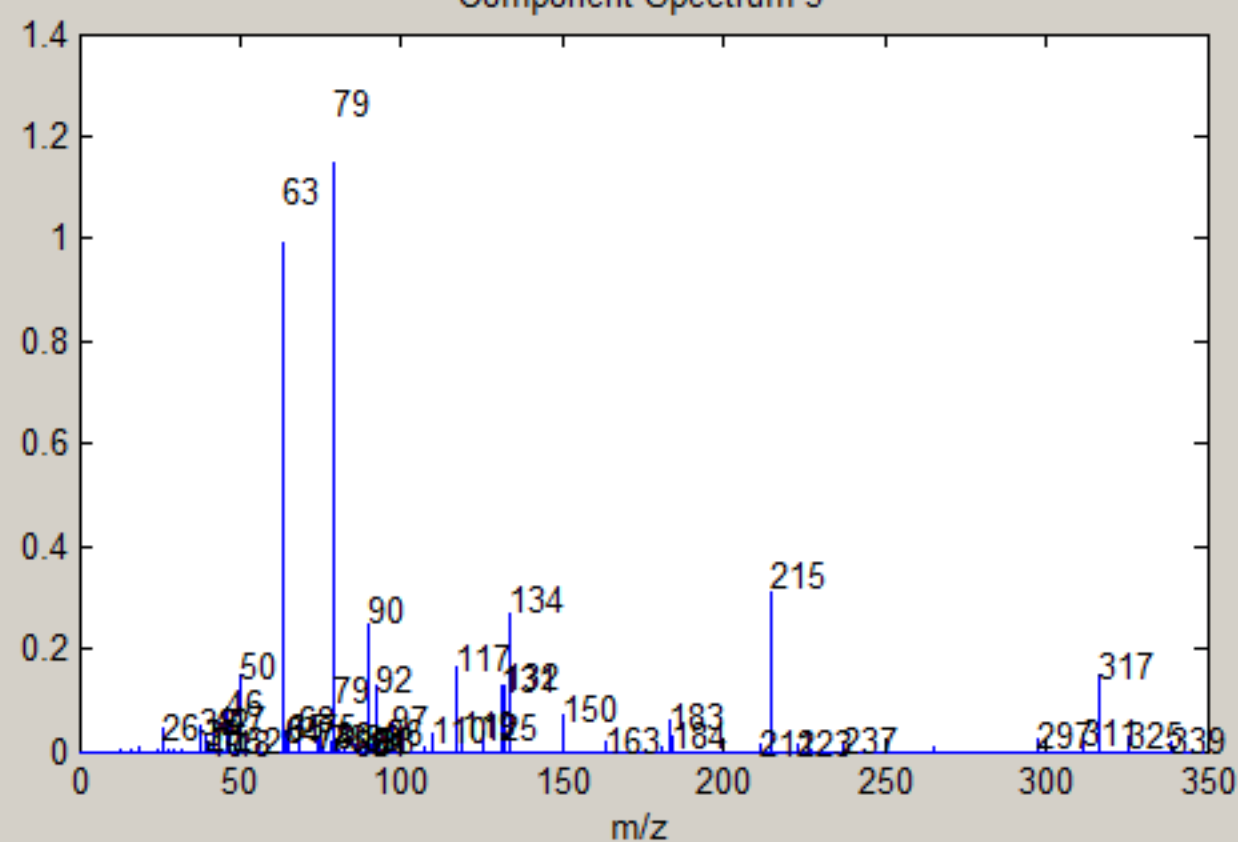
Save Fig

Make Ext

3



Component Spectrum 3



Close panel

Save Component Image as

Save in: MATLAB

Name	Date	Type	Size	Tags
zcorrectorgui	9/6/2013 4:29 PM	File folder		
imagegui	8/23/2013 3:32 PM	File folder		
spectragui	8/23/2013 3:15 PM	File folder		
07_15_13 tripalmitin 18_IonoptikaIA2DspectrV2	7/31/2013 9:41 AM	File folder		
New folder	2/6/2013 10:05 AM	File folder		
slices	2/6/2013 9:57 AM	File folder		
Nick	2/6/2013 9:55 AM	File folder		
correlationsummary.txt	9/16/2013 4:00 PM	Text Document	6 KB	
tiledatatable.txt	7/12/2013 3:58 PM	Text Document	39 KB	
default.txt	6/14/2013 1:31 PM	Text Document	1 KB	
ROIareatable_LOS3tile4.txt	4/9/2013 10:13 AM	Text Document	6 KB	
slice2spot2test.txt	4/5/2013 2:49 PM	Text Document	7 KB	
ROIareatable_fromPCAScores.txt	4/3/2013 3:30 PM	Text Document	8 KB	
test_spot1_pos_NoSilicon.txt	3/11/2013 2:41 PM	Text Document	123 KB	
cottonnegatif2.txt	3/4/2013 8:57 AM	Text Document	3 KB	
MDXWTposALL.txt	2/12/2013 3:11 PM	Text Document	949 KB	
Computer - Shortcut	2/6/2013 9:58 AM	Shortcut	1 KB	
mcrcompspectra.txt	1/30/2013 11:40 AM	Text Document	2,050 KB	
mcrcompimg.txt	1/30/2013 11:40 AM	Text Document	2,050 KB	
mcrcomps.txt	1/30/2013 11:34 AM	Text Document	2,050 KB	
testimage.txt	1/15/2013 9:20 AM	Text Document	1,418 KB	

File name: MCRimagedata

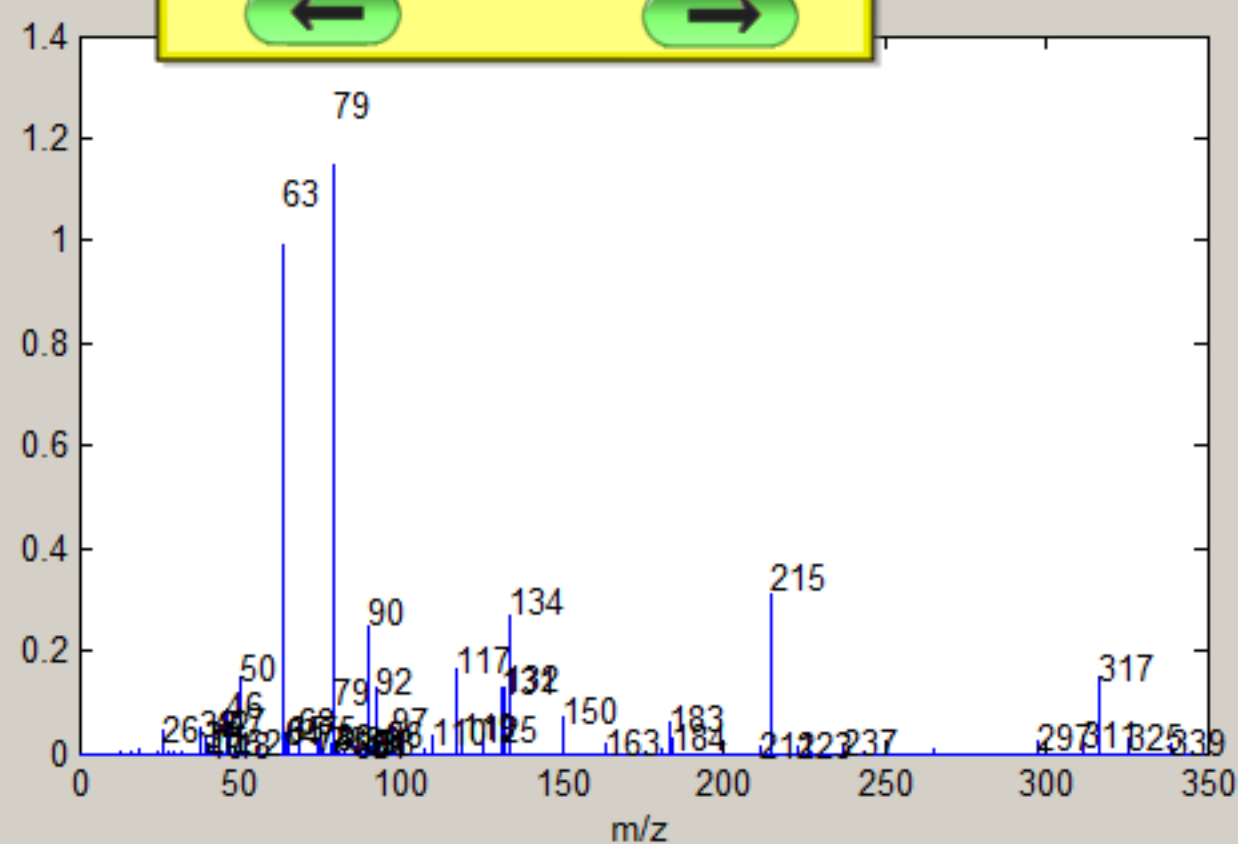
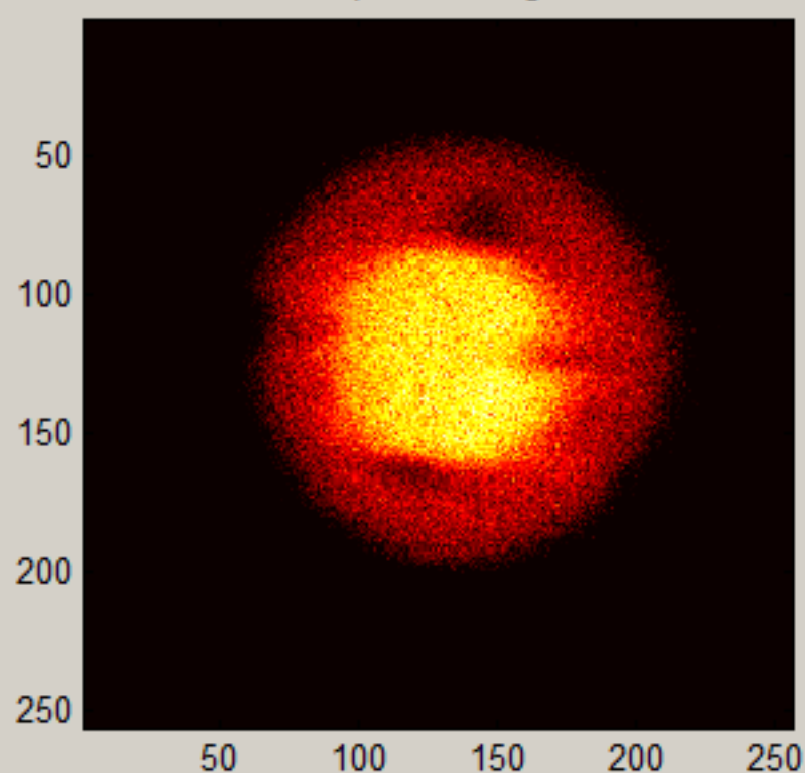
Save as type: tab delimited text (*.txt)

Save

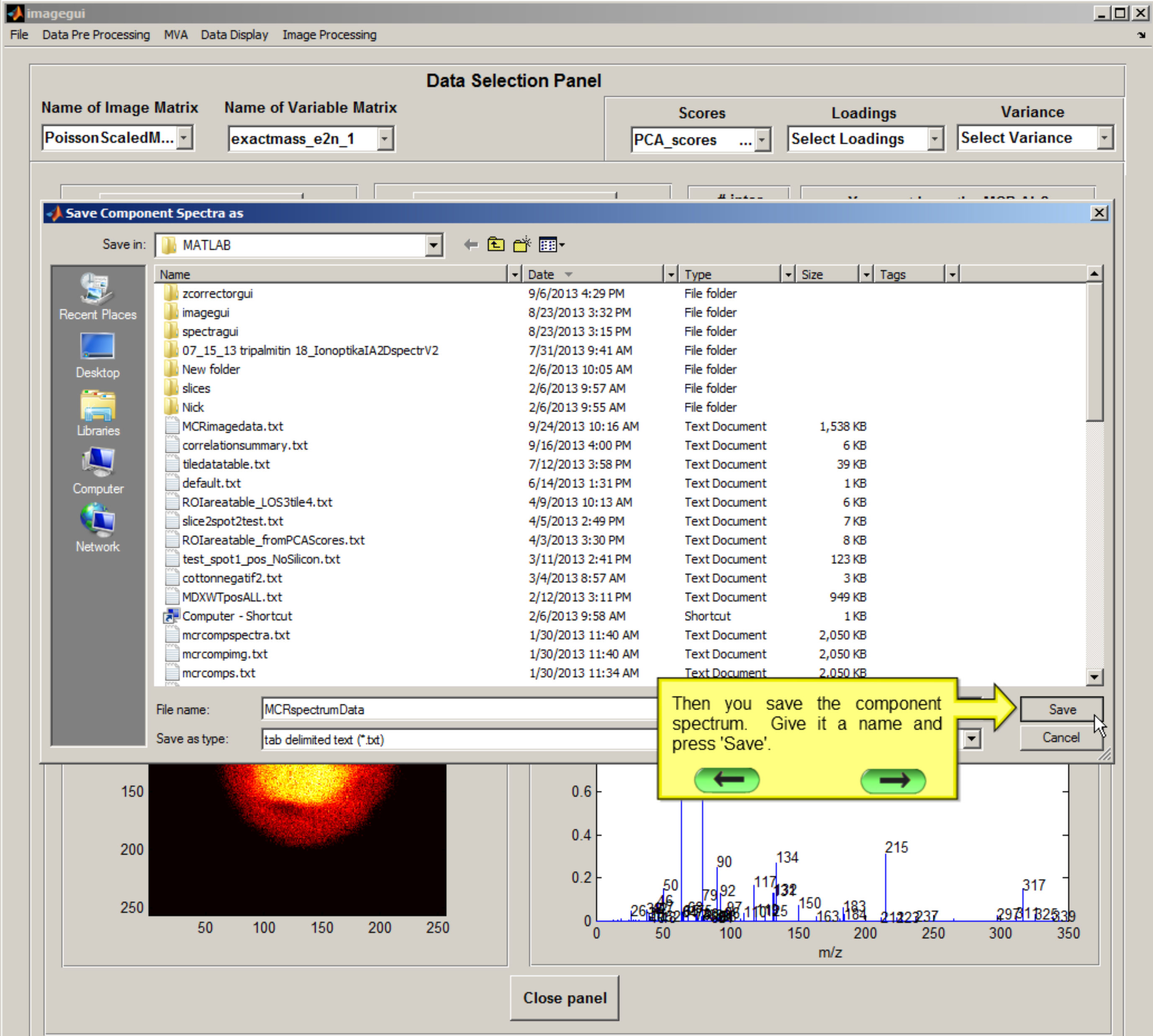
Cancel

First you save the component image. Give it a name and press the 'Save' Button.

Component Image 3



Close panel



Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

PoissonScaledM...

exactmass_e2n_1

Scores

Loadings

Variance

PCA_scores ...

Select Loadings

Select Variance

Load Selected Data

Load Selected Scores

inter

10

Tol.

0.1

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For more information about MCR and the MCR-ALS program, visit the MCR-ALS website. You can access it by pressing the 'Visit MCR-ALS Website' button.

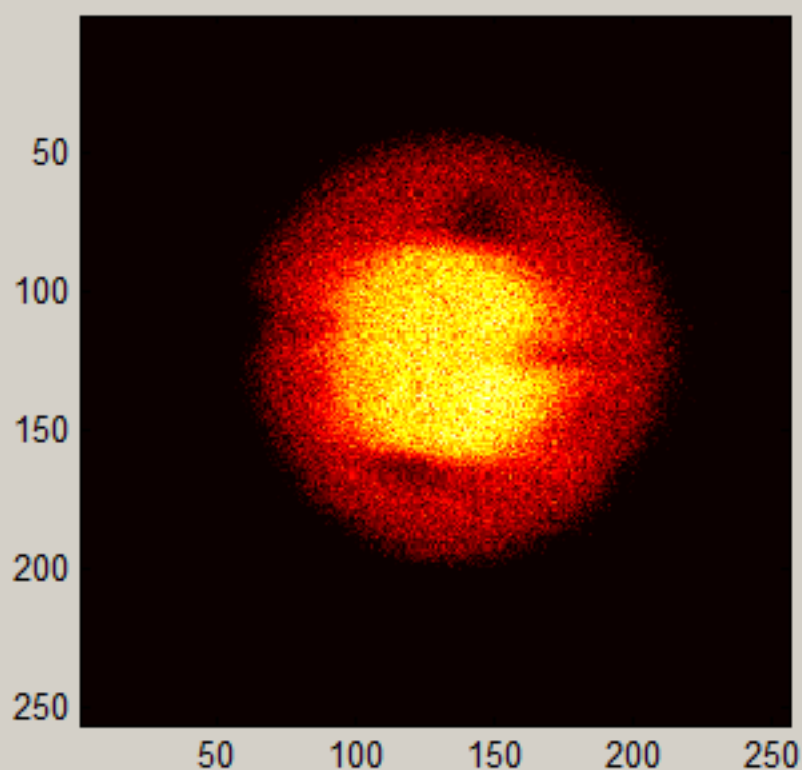
Special thanks to Roma Tauler and Anna de Juan for making their code available for use.

3

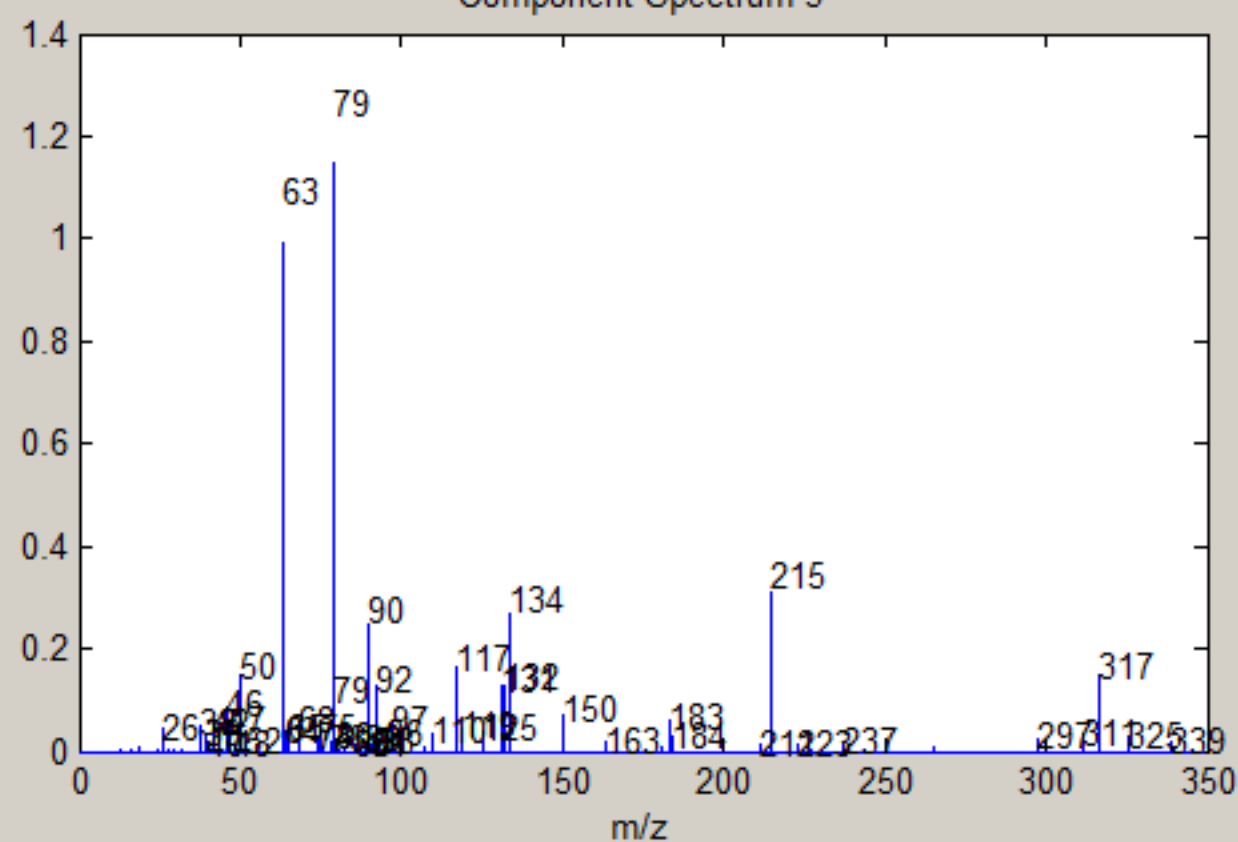
Plot Sel Co

Make Ext

Component Image 3



Component Spectrum 3



Close panel

Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

PoissonScaledM...

exactmass_e2n_1

Scores

Loadings

Variance

PCA_scores ...

Select Loadings

Select Variance

Load Selected Data

Load Selected Scores

inter

10

Tol.

0.1

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Run MCR

Save MCR Results

3

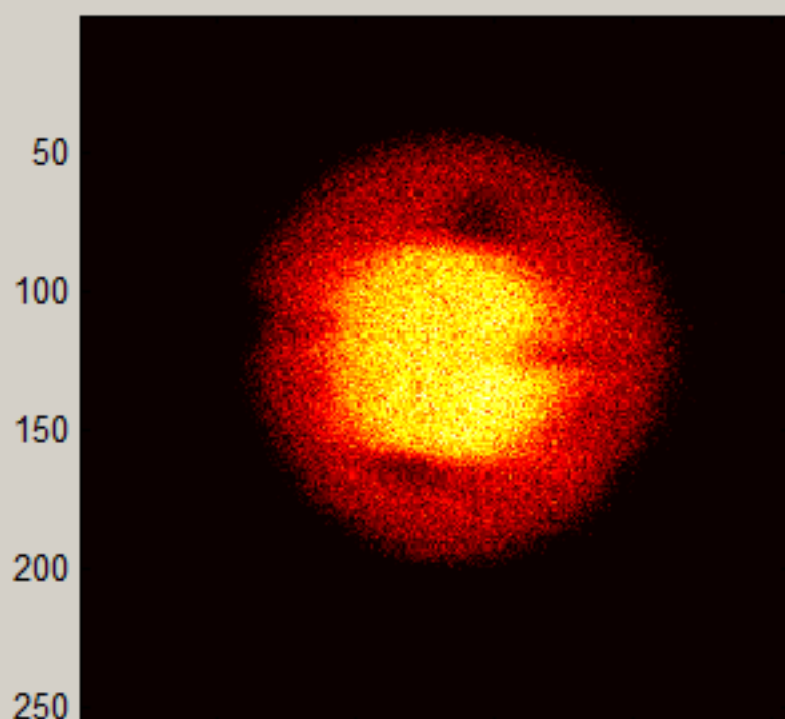
Plot Sel Comp

Plot All Comp

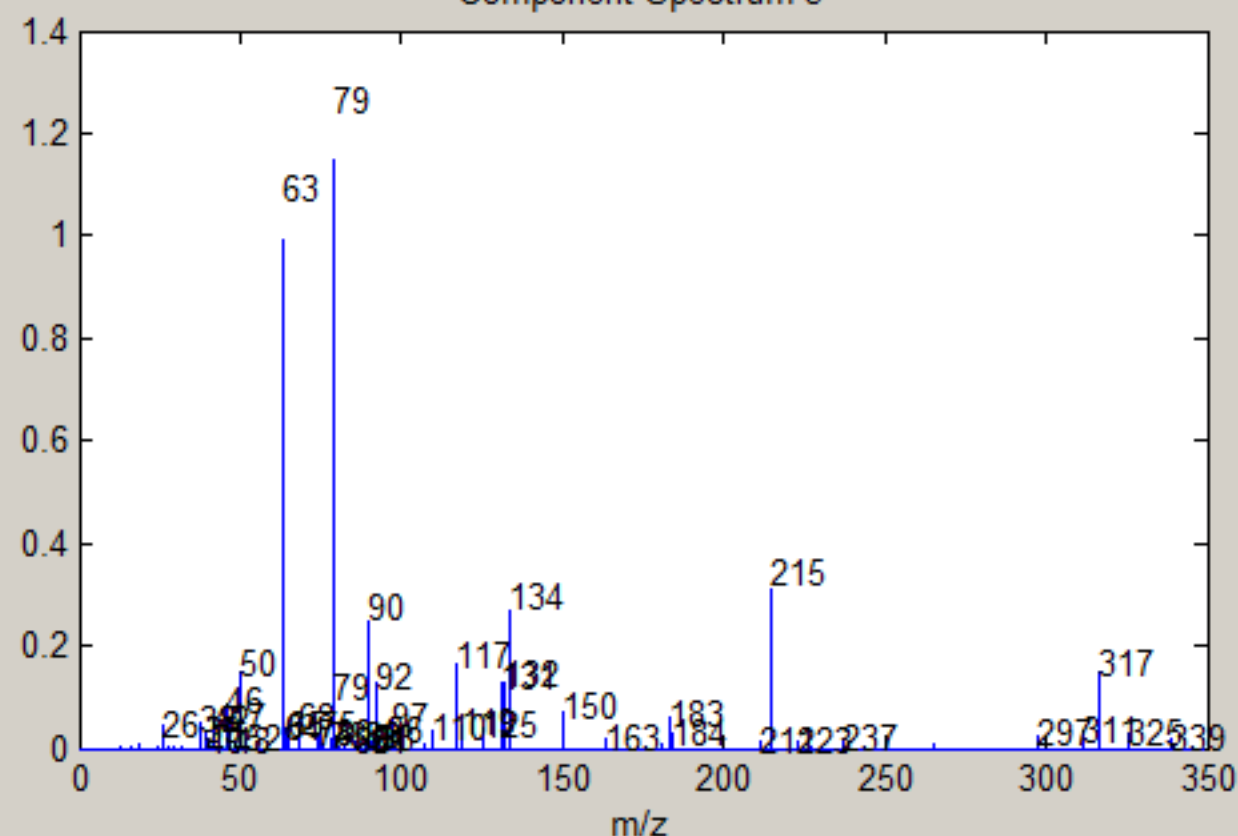
Save Fig

Make Ext

Component Image 3



Component Spectrum 3



Close the panel by pressing the 'Close panel' button.

Close panel

Data Selection Panel

Name of Image Matrix

Poisson ScaledM...

Name of Variable Matrix

exactmass_e2n_1

Scores

PCA_scores ...

Loadings

Select Loadings

Variance

Select Variance

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.

