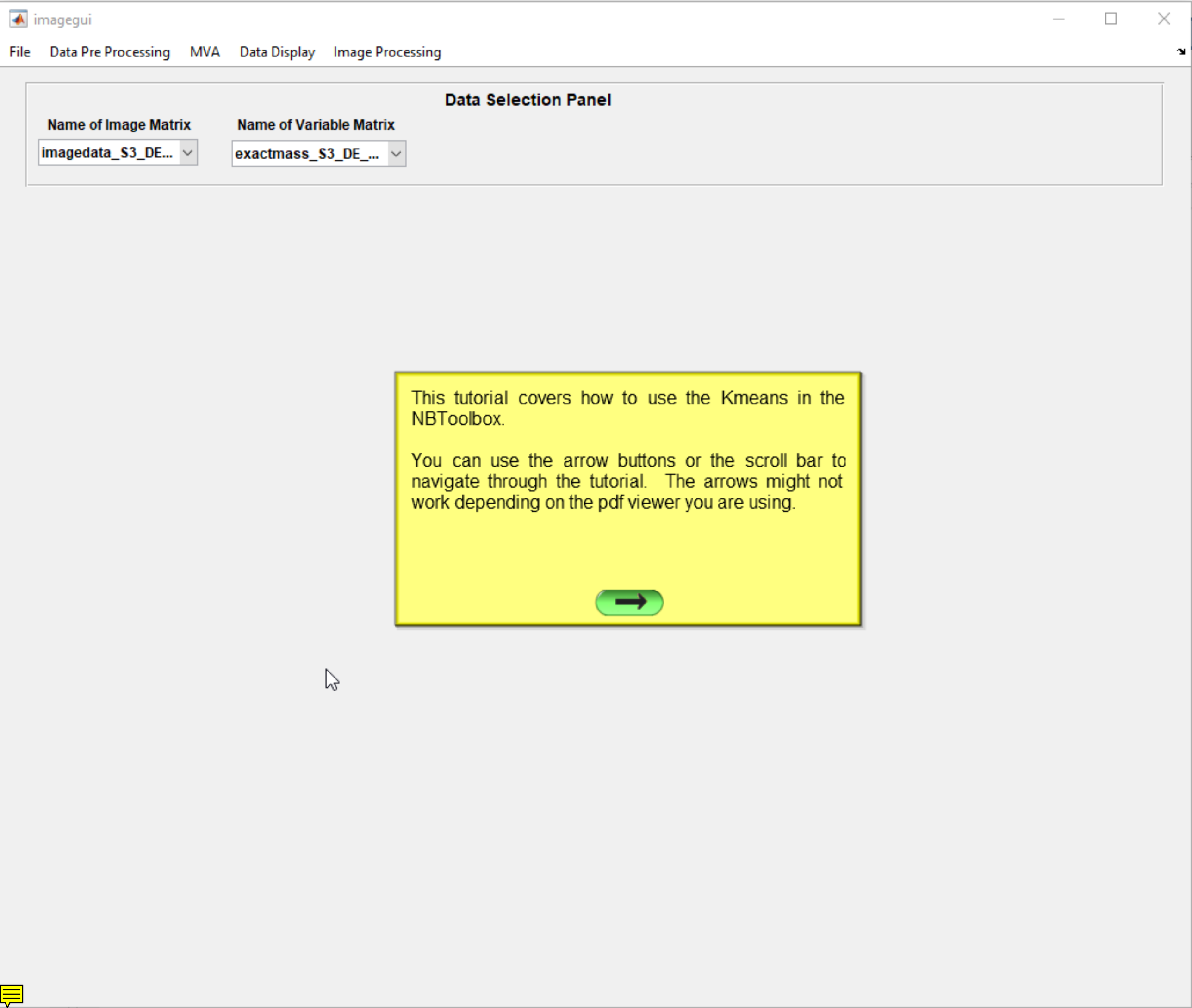
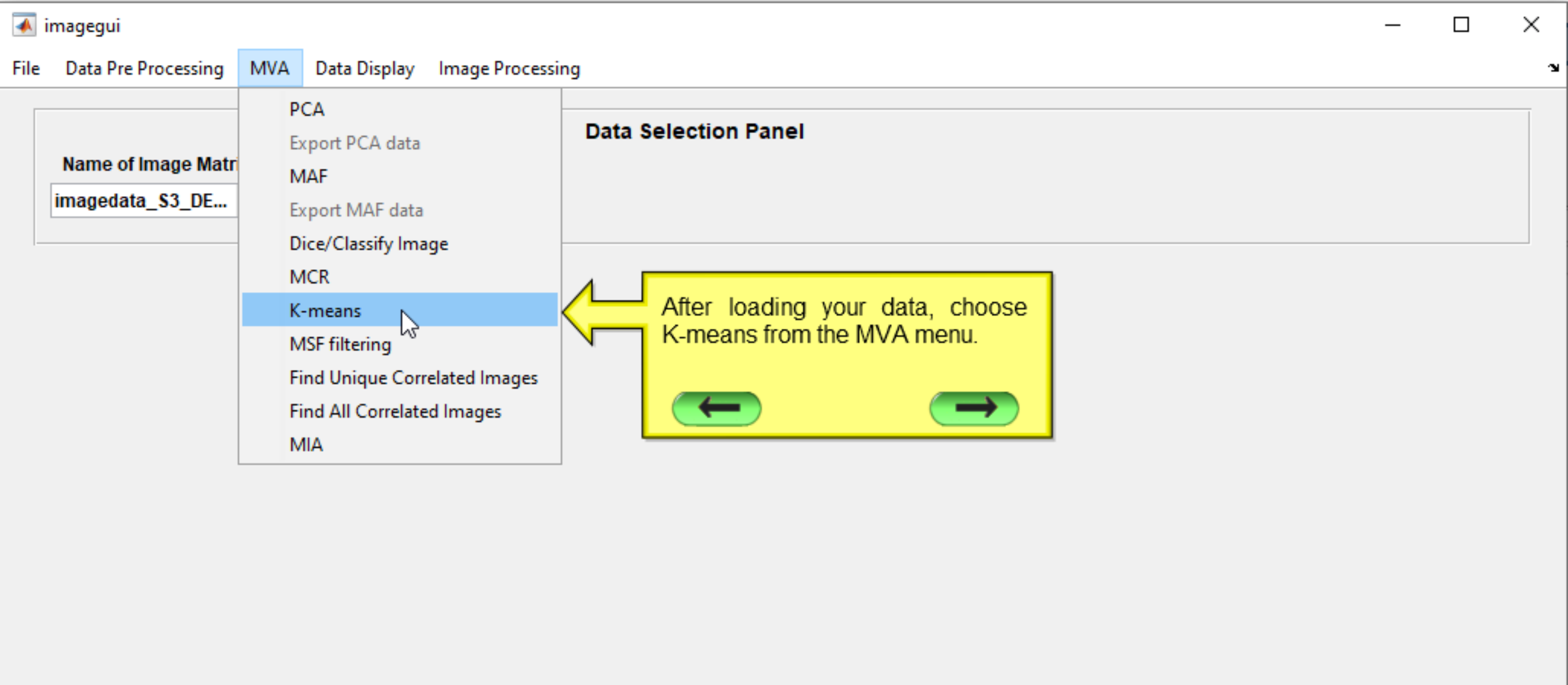

imagegui
File
Data Pre Processing
MVA
Data Display
Image Processing
Data Selection Panel
Name of Image Matrix
imagedata_S3_DE...
Name of Variable Matrix
exactmass_S3_DE_...
This tutorial covers how to use the Kmeans in the NBToolbox.
You can use the arrow buttons or the scroll bar to navigate through the tutorial. The arrows might not work depending on the pdf viewer you are using.


imagegui
File
Data Pre Processing
MVA
Data Display
Image Processing
PCA
Export PCA data
MAF
Export MAF data
Dice/Classify Image
MCR
K-means
MSF filtering
Find Unique Correlated Images
Find All Correlated Images
MIA
Name of Image Matr
imagedata_S3_DE...
Data Selection Panel
After loading your data, choose K-means from the MVA menu.

imagegui

File Data Pre Processing MVA Data Display Image Processing

Data Selection Panel

Name of Image Matrix

imagedata_S3_DE...

Name of Variable Matrix

exactmass_S3_DE_...

Load Selected Data

Image: None

Variables: None

Make sure the data you want to process is selected in the Data Selection Panel and press the 'Load Selected Data' button.

Close panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

Data Selection Panel

Name of Image Matrix

imagedata_S3_DE...

Name of Variable Matrix

exactmass_S3_DE_...

Load Selected Data

Image: imagedata_S3_DE_03_1

Variables: exactmass_S3_DE_03_1

Choose distance measure

Choose one...

Number of factors to calculate

Run K-Means

Save K-Means Res...

The loaded data will be shown in red here.

Close panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

Data Selection Panel

Name of Image Matrix: imagedata_S3_DE...

Name of Variable Matrix: exactmass_S3_DE_...

Load Selected Data

Image: imagedata_S3_DE_03_1

Variables: exactmass_S3_DE_03_1

Choose distance measure

Choose one...

- Choose one...
- sqeuclidean
- cityblock
- cosine

Number of factors to

Run K-Means

Choose a distance measure here. The distance measure is the measure minimized by by k-means when determining groups.

'sqeuclidean' - Squared Euclidean distance.

'cityblock' - Sum of absolute differences, a.k.a. L1 distance

'cosine' - One minus the cosine of the included angle between points (treated as vectors).

Here we will use sqeuclidean.

Close panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

Data Selection Panel

Name of Image Matrix: imagedata_S3_DE...

Name of Variable Matrix: exactmass_S3_DE_...

Load Selected Data

Image: imagedata_S3_DE_03_1

Variables: exactmass_S3_DE_03_1

Choose distance measure: sqeuclidean

Choose cluster measure: Choose one...

- Choose one...
- cluster
- plus
- sample
- uniform

Number of factors to calculate

Run K-Means

This is the method use to determine the initial cluster centers.

'cluster' - Perform preliminary clustering phase on random 10% subsample of X.

'plus' - Select K observations from X according to the k-means++ algorithm: the first cluster center is chosen uniformly at random from X, after which each subsequent cluster center is chosen randomly from the remaining data points with probability proportional to its distance from the point's closest existing cluster center.

'sample' - Select K observations from X at random.

'uniform' - Select K points uniformly at random from the range of X.

Here we will use cluster.

Close panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

Data Selection Panel

Name of Image Matrix

imagedata_S3_DE...

Name of Variable Matrix

exactmass_S3_DE_...

Load S

Image: in

Variables: e

Choose the number of factors to calcuate. This should be chosen based on the number of suspected components in the system.

K-means will always calculate the number of factors you specify. It is up to you to determine if the calculated factors contain real and useful information.

Number of factors to calculate 3

Run K-Means

Number of iterations

Save K-Means Res...

Close panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

Data Selection Panel

Name of Image Matrix

imagedata_S3_DE...

Name of Variable Matrix

exactmass_S3_DE_...

Load Selected Data

Image: image

Variables: exactm

Choose distance measure

sqeuclidean

Choose the number of iterations to use for the calculation. More iterations will take longer and may not provide "better" results.

Number of factors to calculate 3

Run K-Means

Number of iterations 5

Save K-Means Res...

Close panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

Data Selection Panel

Name of Image Matrix

imagedata_S3_DE...

Name of Variable Matrix

exactmass_S3_DE_...

Load Selected Data

Image: imagedata_S3_DE_03_1

Variables: exactmass_S3_DE_03_1

Choo

sqe

Cho

clu

Press the Run K-Means button to start the function.

Run K-Means

5

Save K-Means Res...

Close panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

Data Selection Panel

Name of Image Matrix: imagedata_S3_DE...

Name of Variable Matrix: exactmass_S3_DE_...

Load Selected Data

Image: imagedata_S3_DE_03_1

Variables: exactmass_S3_DE_03_1

Choose distance measure: sqeuclidean

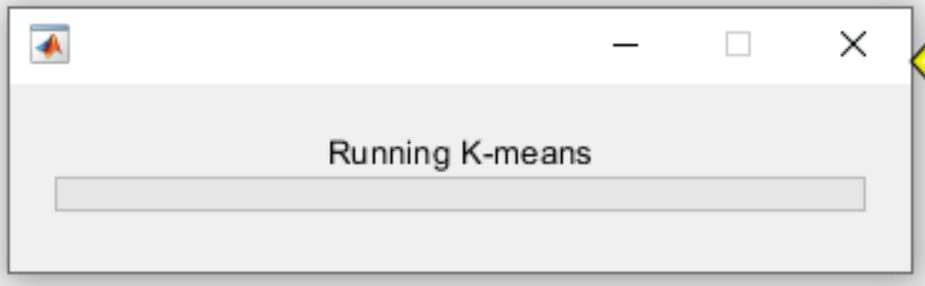
Choose cluster measure: cluster

Number of factors to calculate: 3

Number of iterations: 5

Run K-Means

Save K-Means Res...



The processing bar will open up and disappear when the calculations are complete.

Close panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

Data Selection Panel

Name of Image Matrix: imagedata_S3_DE...

Name of Variable Matrix: exactmass_S3_DE_...

Load Selected Data

Image: imagedata_S3_DE_03_1

Variables: exactmass_S3_DE_03_1

Choose distance measure: sqeuclidean

Choose cluster measure: cluster

Number of factors to calculate: 3

Number of iterations: 5

Run K-Means

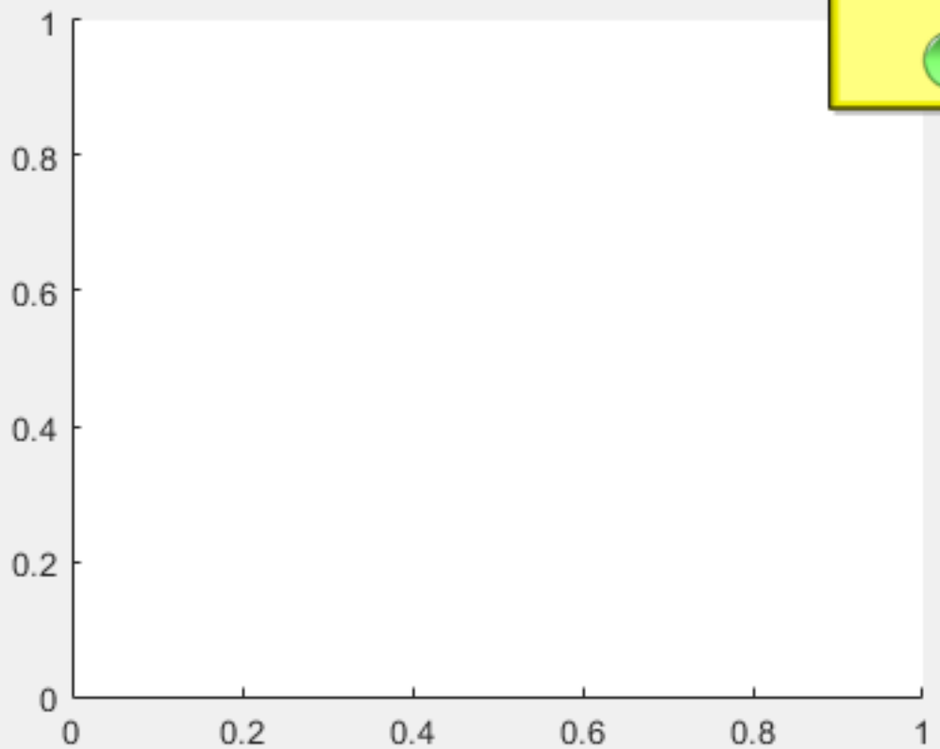
Save K-Means Res...

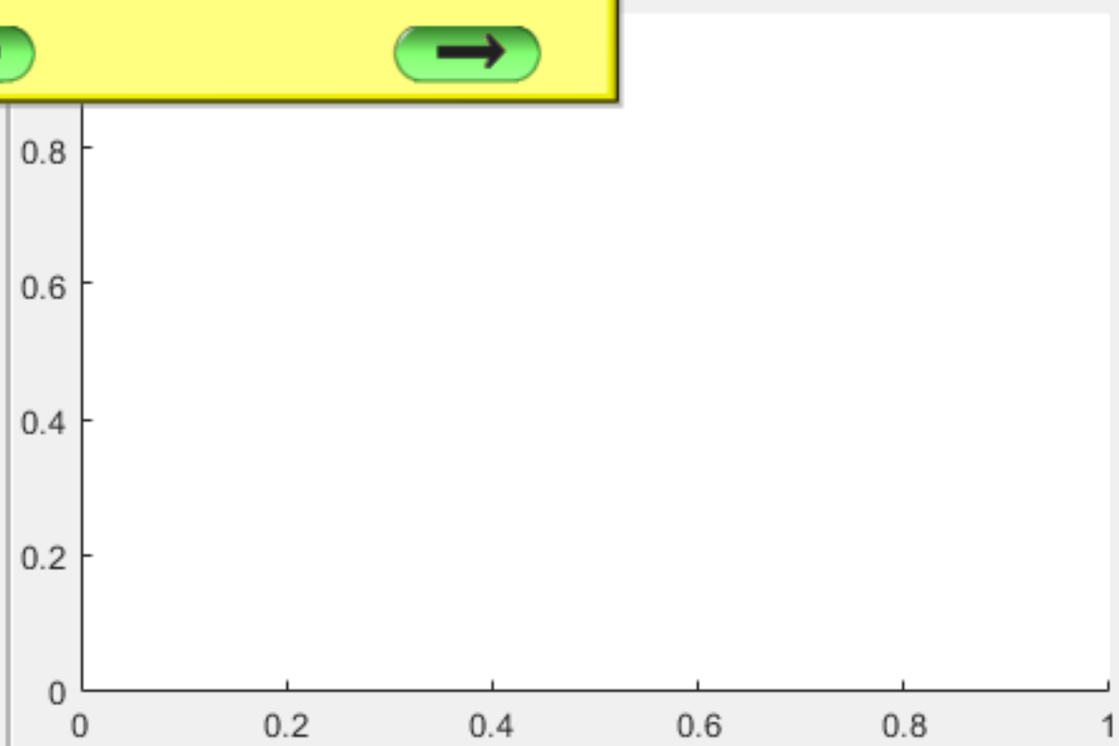
Choose component #

Choose component #
1
2
3

Plot Sel Comp Plot All Comp Save Fig Make Ext

Once the calculations are complete, you can select a component from the drop down menu and then look at the results.





Close panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

Data Selection Panel

Name of Image Matrix: imagedata_S3_DE...

Name of Variable Matrix: exactmass_S3_DE_...

Load Selected Data

Image: imagedata_S3_DE_03_1

Variables: exactmass_S3_DE_03_1

Choose distance measure: sqeuclidean

Choose cluster measure: cluster

Number of factors to calculate: 3

Number of iterations: 5

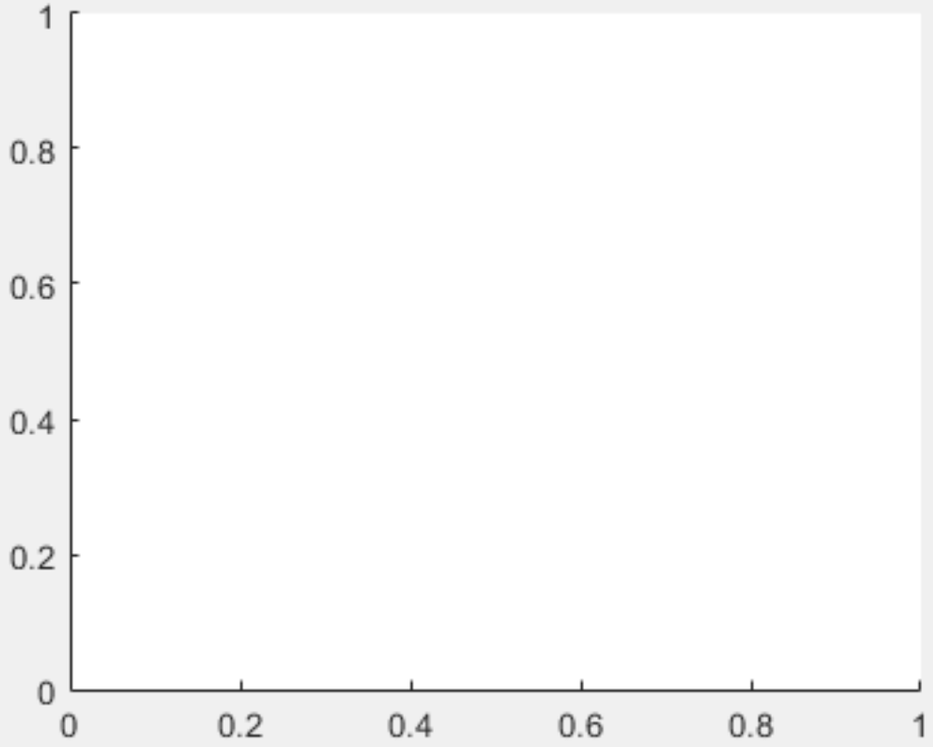
Run K-Means

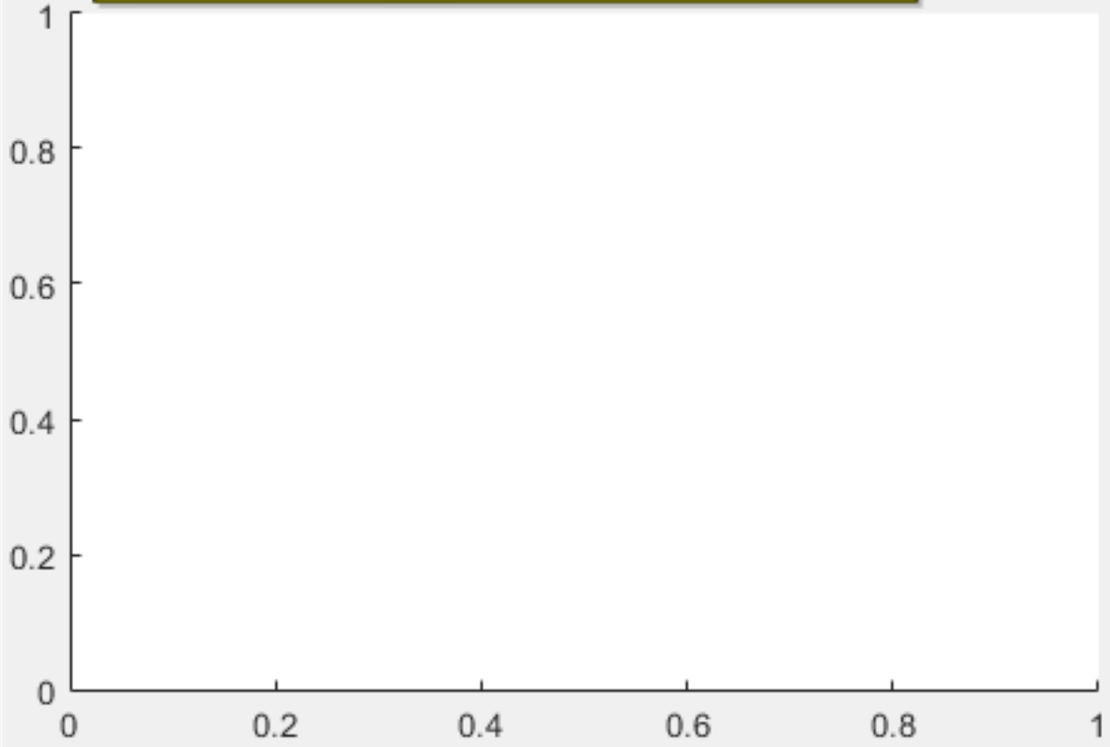
Save K-Means Res...

1

Plot Sel Comp

Press the Plot Sel Comp button to see the component image and calculated factor spectrum.





Close panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

Data Selection Panel

Name of Image Matrix: imagedata_S3_DE...

Name of Variable Matrix: exactmass_S3_DE_...

Load Selected Data

Image: imagedata_S3_DE_03_1

Variables: exac

Choose distance measure: sqeuclidean

Choose cluster measure

Number of factors to calculate: 3

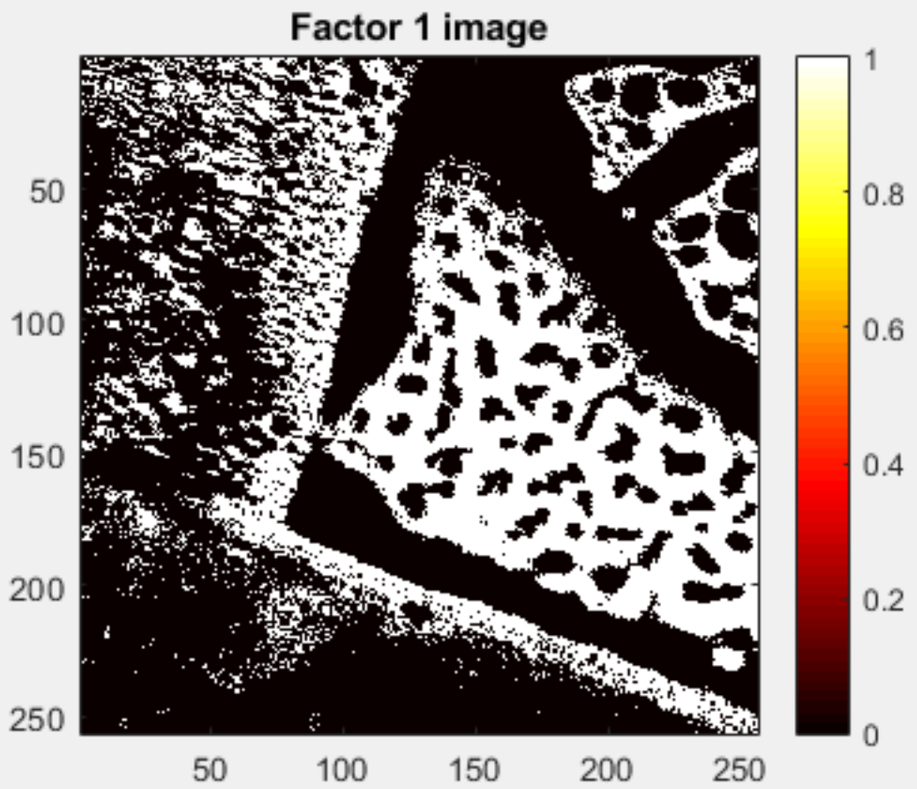
Number of iterations: 5

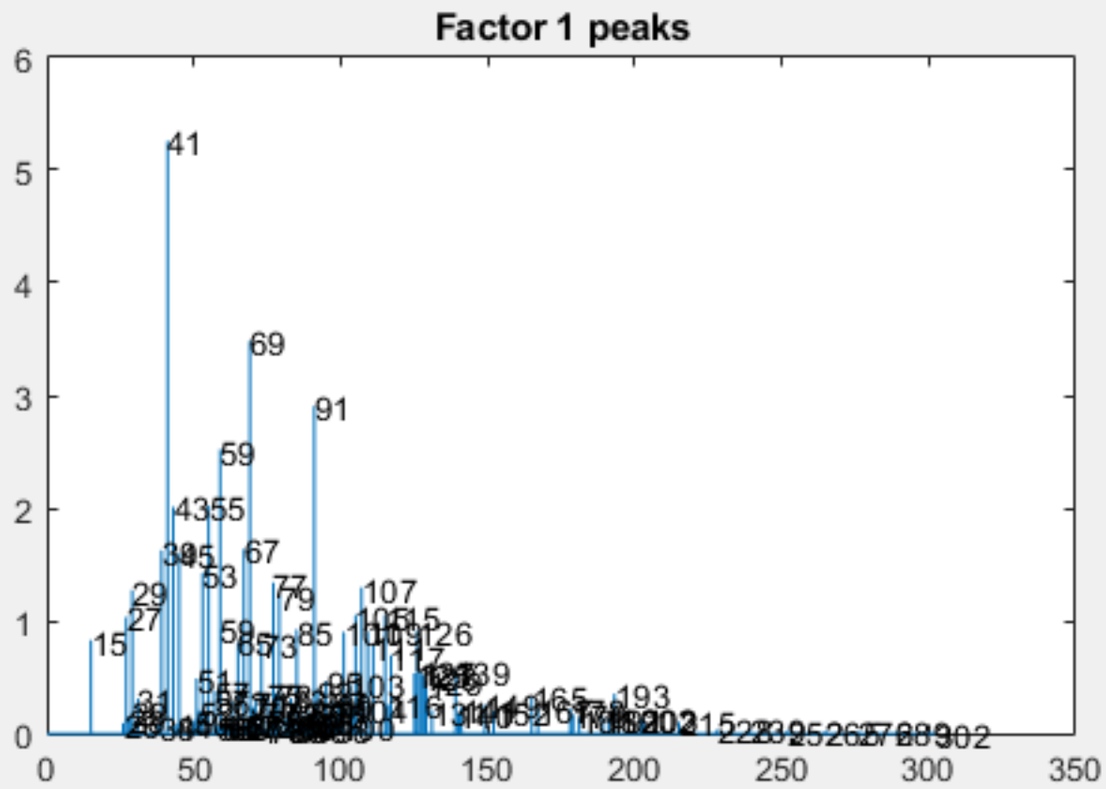
Run K-Means

Save K-Means Res...

The component image and calculated factor spectrum will appear in these plots.

l Comp Save Fig Make Ext





Close panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

Data Selection Panel

Name of Image Matrix: imagedata_S3_DE...

Name of Variable Matrix: exactmass_S3_DE_...

Load Selected Data

Image: imagedata_S3_DE_03_1

Variables: exactmass_S3_DE_03_1

Choose distance measure: sqeuclidean

Choose cluster measure: cluster

Number of factors to calculate: 3

Number of iterations: 5

Run K-Means

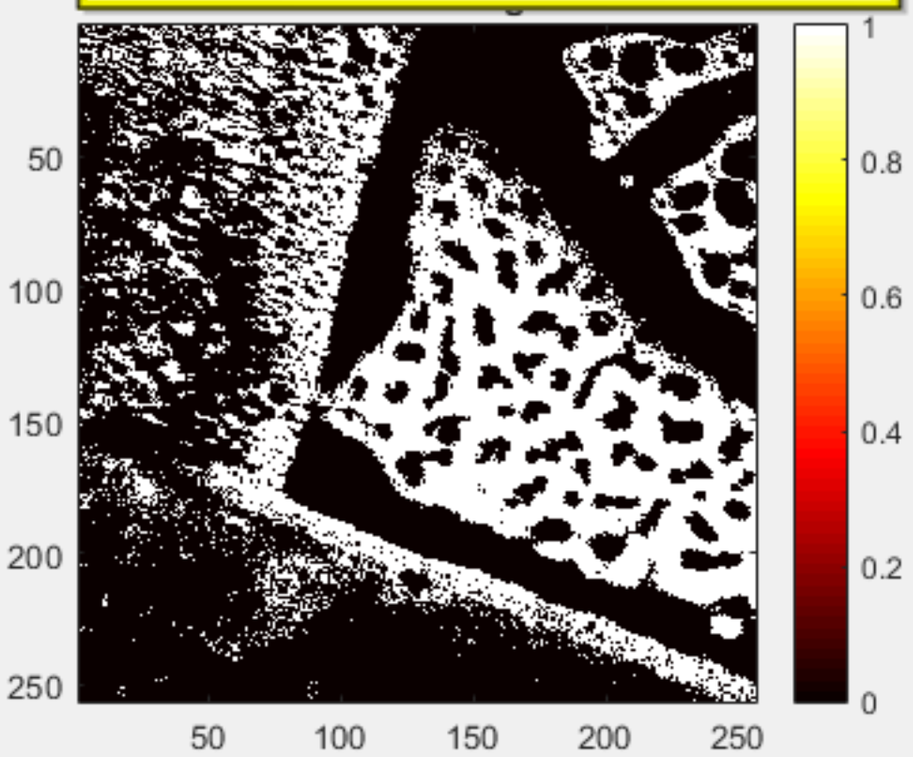
Save K-Means Res...

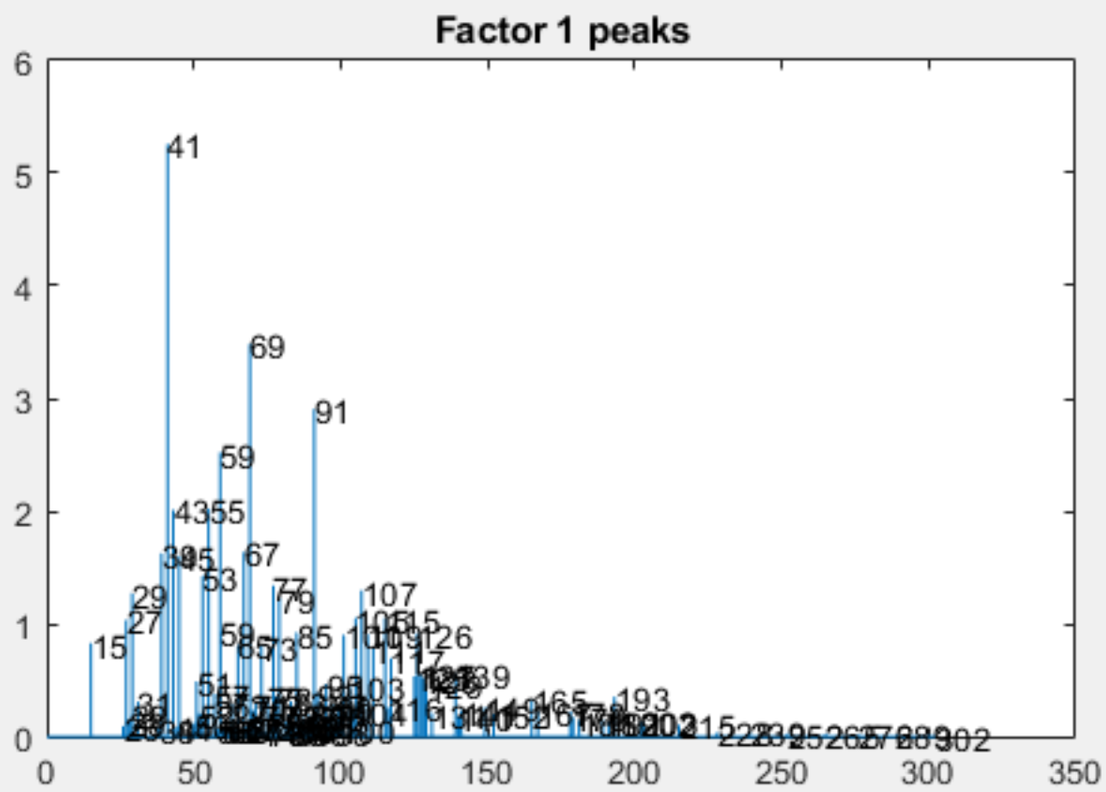
Press the Plot All Comp buttons to create separete figures for all components.

Plot All Comp

Save Fig

Make Ext





Close panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

Data Selection Panel

Name of Image Matrix **Name of Variable Matrix**

imagedata_S3_DE...

Load Sele

Image: imag

Variables: exact

Figure 6

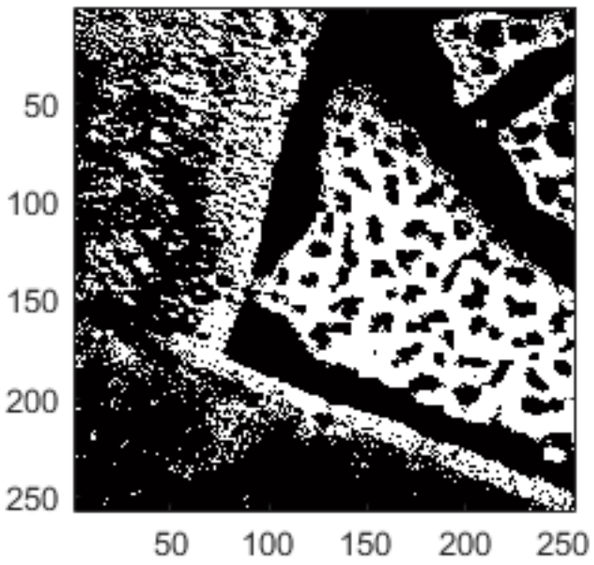
Figure 4

File File Edit Vi

Figure 3

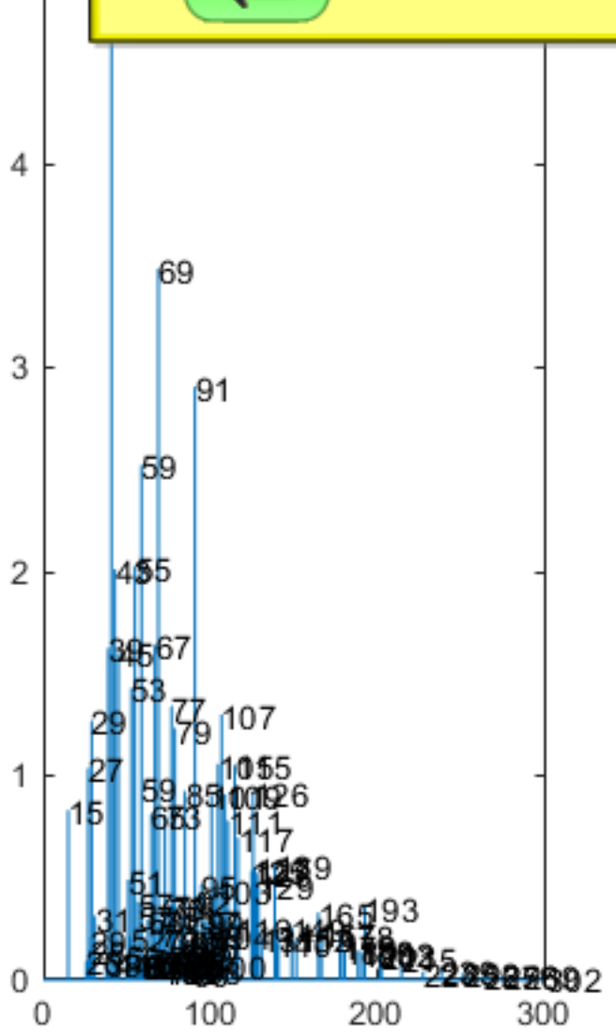
File Edit View Insert Tools Desktop Window Help

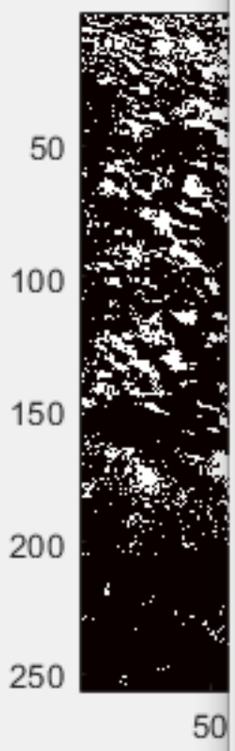
Factor 1 image

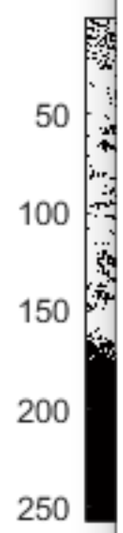


Factor 1 peaks

A figure will be created for each component showing the component image and spectrum.







se panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

Data Selection Panel

Name of Image Matrix **Name of Variable Matrix**

imagedata_S3_DE...

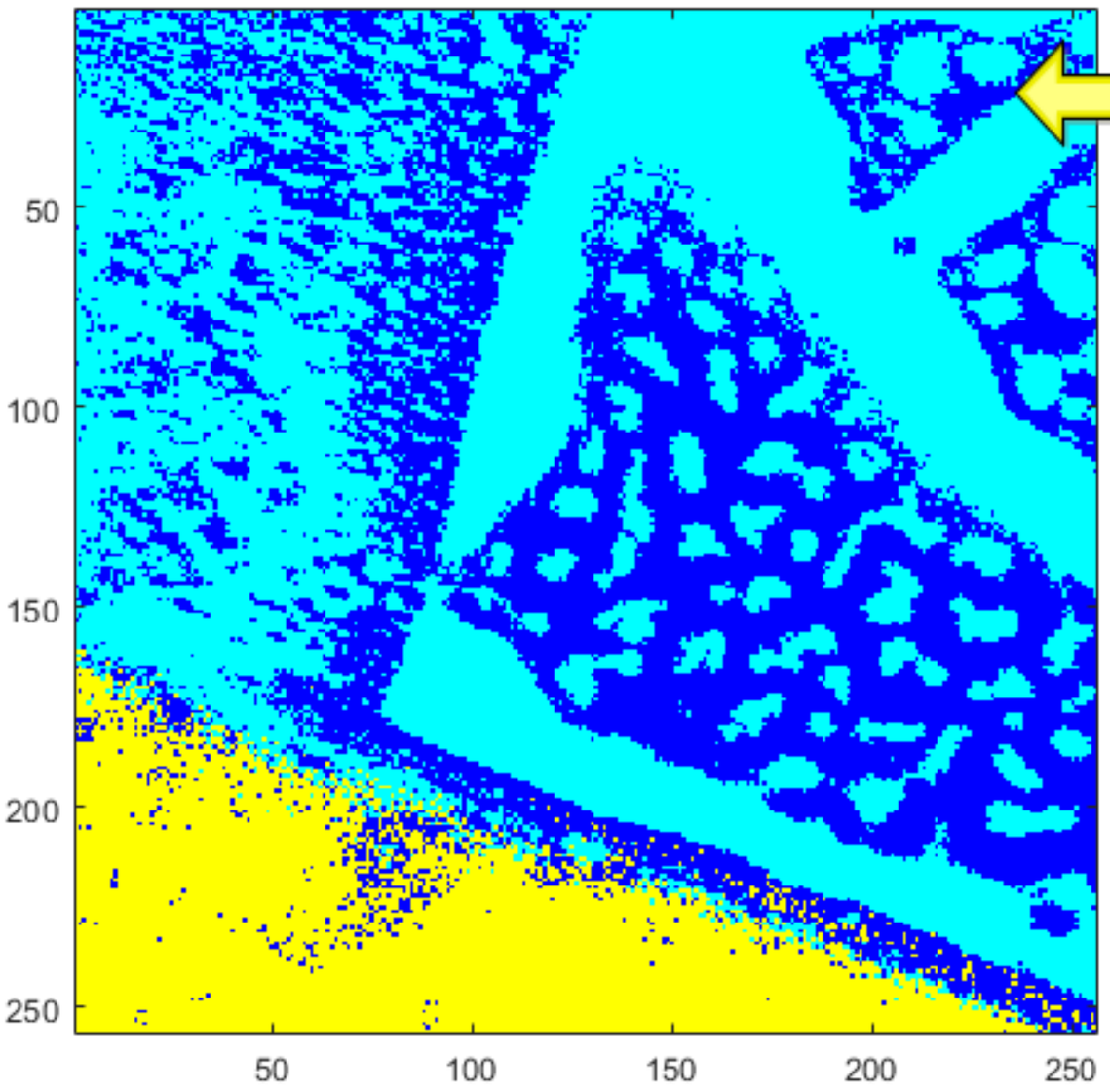
Load Sele

Image: imag

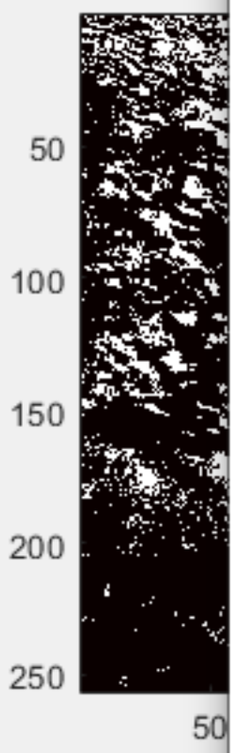
Variables: exact

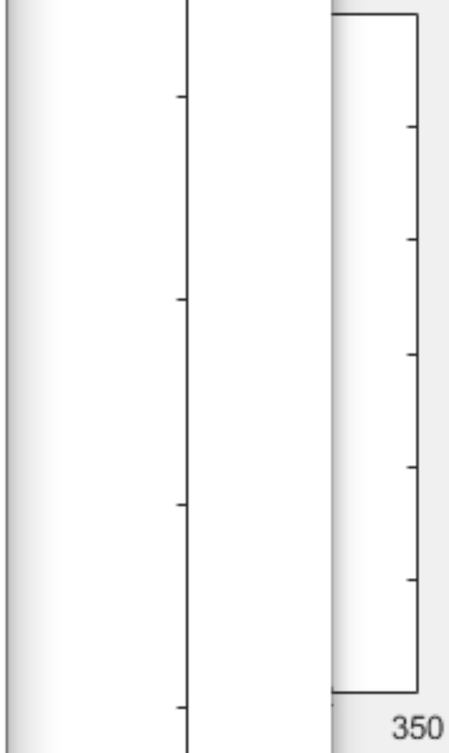
Figure 6

File Edit View Insert Tools Desktop Window Help



An image showing an overlay of all components will also be created.





se panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

Data Selection Panel

Name of Image Matrix: imagedata_S3_DE...

Name of Variable Matrix: exactmass_S3_DE_...

Load Selected Data

Image: imagedata_S3_DE_03_1

Variables: exactmass_S3_DE_03_1

Choose distance measure: sqeuclidean

Choose cluster measure: cluster

Number of factors to calculate: 3

Number of iterations: 5

Run K-Means

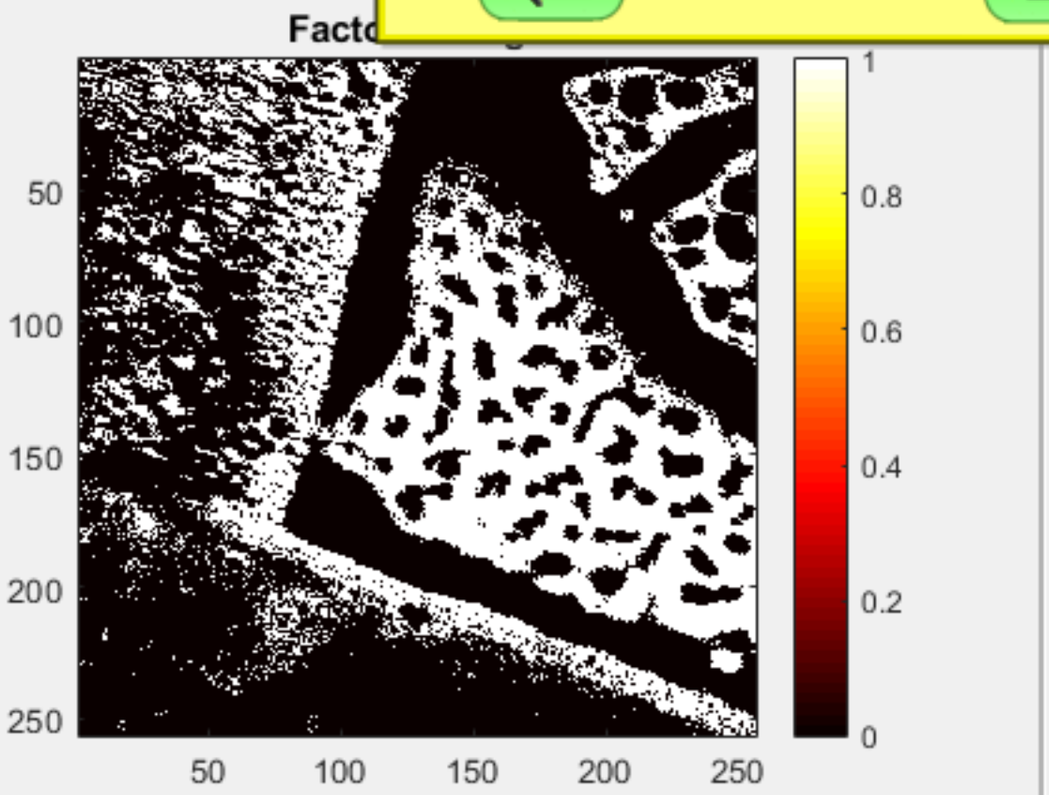
Save K-Means Res...

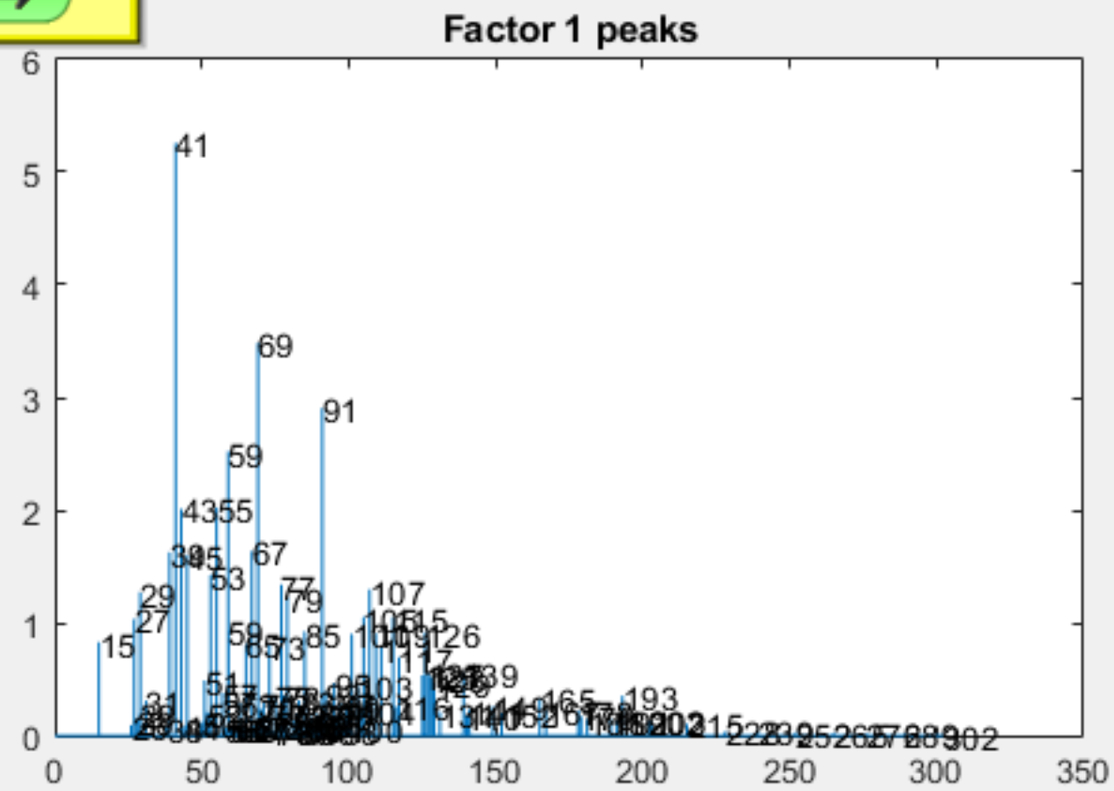
1

Press the Save Fig button to save the data shown in the plotten figures below.

Save Fig

Make Ext





Close panel

imagegui

Save Component Image as

This PC › Documents › MATLAB ›

Search MATLAB

Organize New folder

MATLAB
pngfiles
SpectraFiles
Summary
OneDrive
This PC
3D Objects
Desktop
Documents
Custom Office Templates
Fax
MATLAB

Name	Date
A2DP02_Correlation	3/30/2022 10:48 AM
A1DP02_Correlation	3/30/2022 10:45 AM
NFigA01.jpg	5/31/2024 4:46 PM
RPMMA-GPEG-BPS.jpg	3/29/2024 1:53 PM
kmsspec1.jpg	3/15/2024 11:28 AM
kmscom1.jpg	3/15/2024 11:28 AM
AAPANEg-mixconprojectedintoConModel.jpg	11/3/2023 4:39 PM
test_rock2image.jpg	3/9/2023 4:36 PM
MM3CDP-regularization.jpg	9/2/2022 3:31 PM
default.jpg	9/1/2022 3:26 PM
Cs30Br10_27_9_Si_Unfolded.jpg	7/14/2022 4:14 PM
Cs30Br10_27_9_Si.jpg	7/14/2022 4:13 PM

File name: KmeansComponent1.jpg

Save as type: jpeg (*.jpg)

Hide Folders

Save Cancel

A dialog box will open asking you for a name for the component image and then one asking for a name for the component spectrum.

-Means

Means Res...

Ext

Close panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

Data Selection Panel

Name of Image Matrix: imagedata_S3_DE...

Name of Variable Matrix: exactmass_S3_DE_...

Load Selected Data

Image: imagedata_S3_DE_03_1

Variables: exactmass_S3_DE_03_1

Choose distance measure: sqeuclidean

Choose cluster measure: cluster

Number of factors to calculate: 3

Number of iterations: 5

Run K-Means

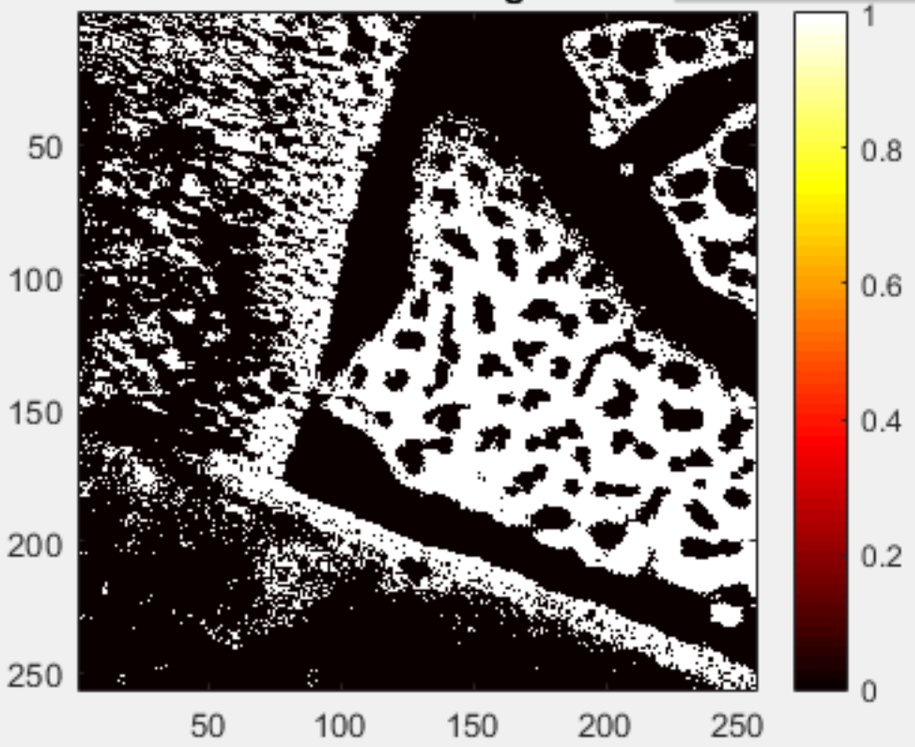
Save K-Means Res...

1

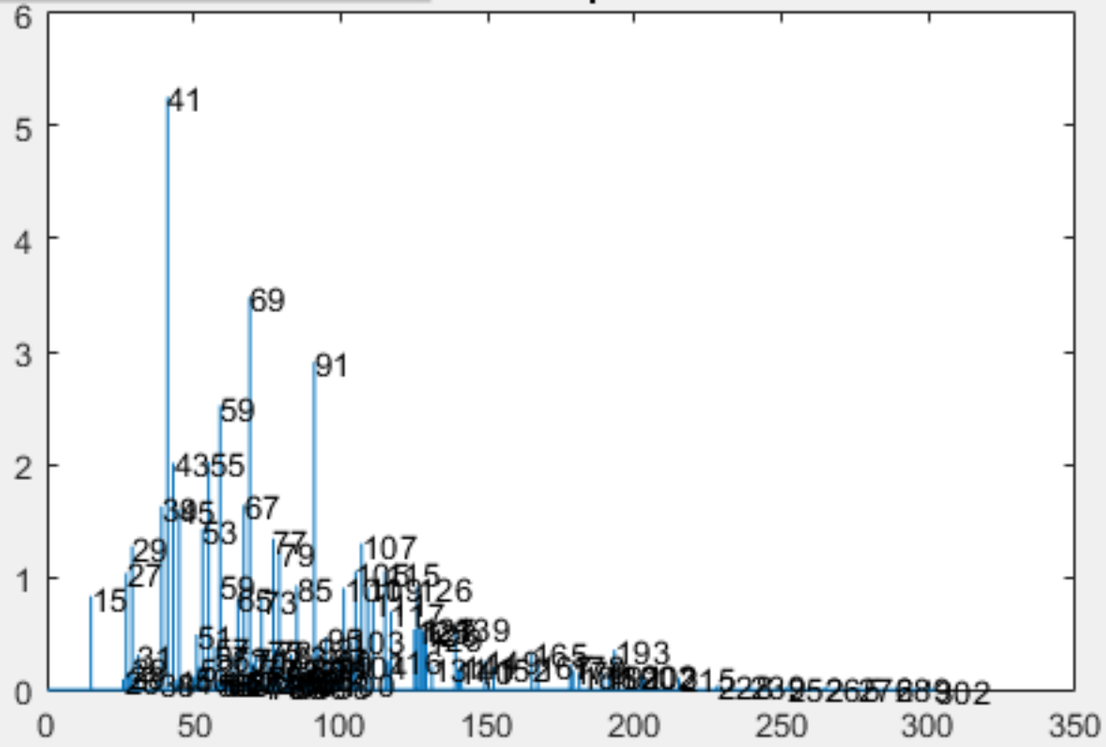
Press the Make Ext button to create standalone figures for the component data displayed in the panel.

Make Ext

Factor 1 image



Factor 1 peaks



Close panel

imagegui

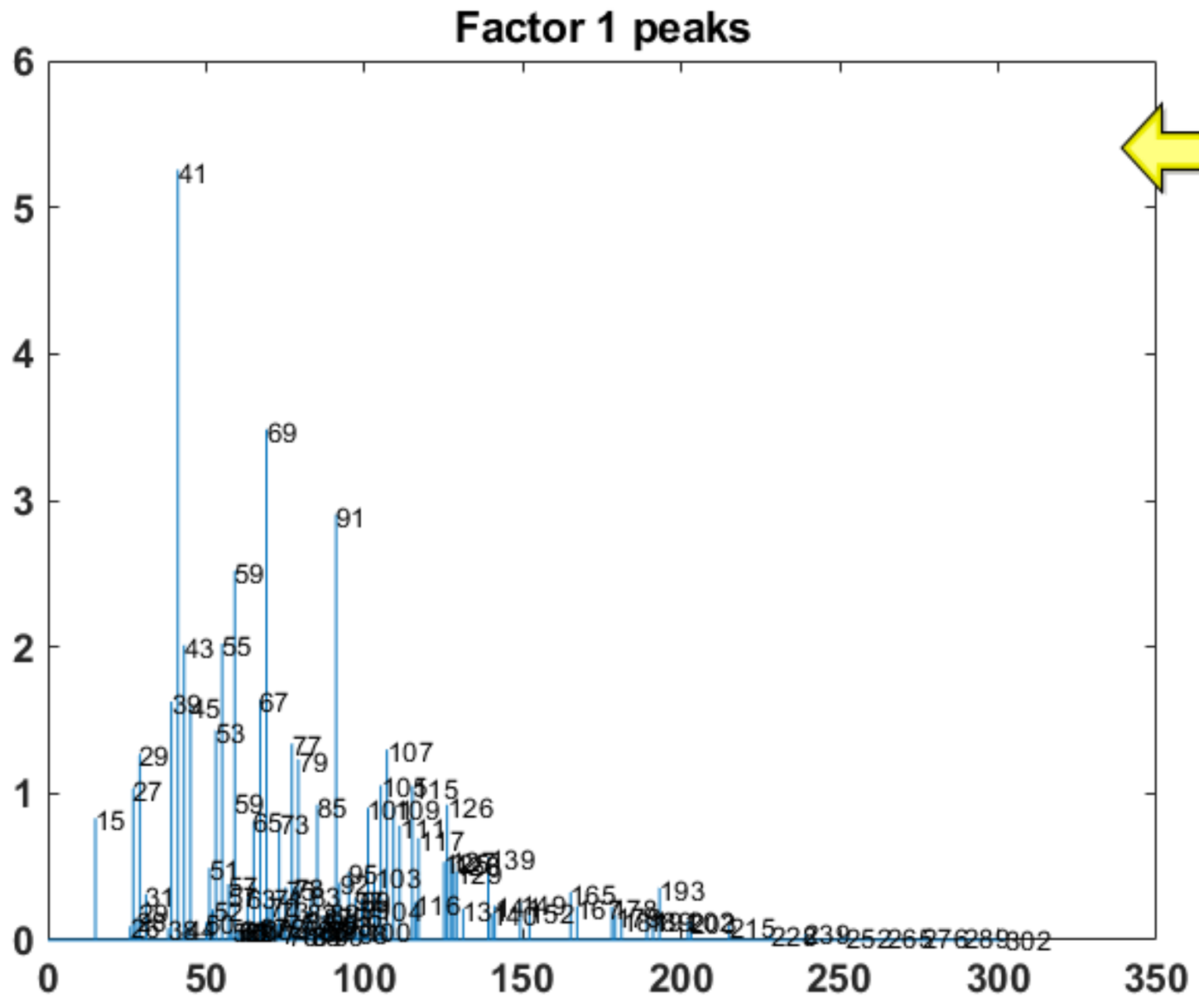
File Data Pre Processing MVA Data Display Image Processing

Data Selection Panel

Name of Image Matrix **Name of Variable Matrix**

Figure 6

File Edit View Insert Tools Desktop Window Help



Desktop Window Help

A figure will be created showing the component spectrum.

imagegui

File Data Pre Processing MVA Data Display Image Processing

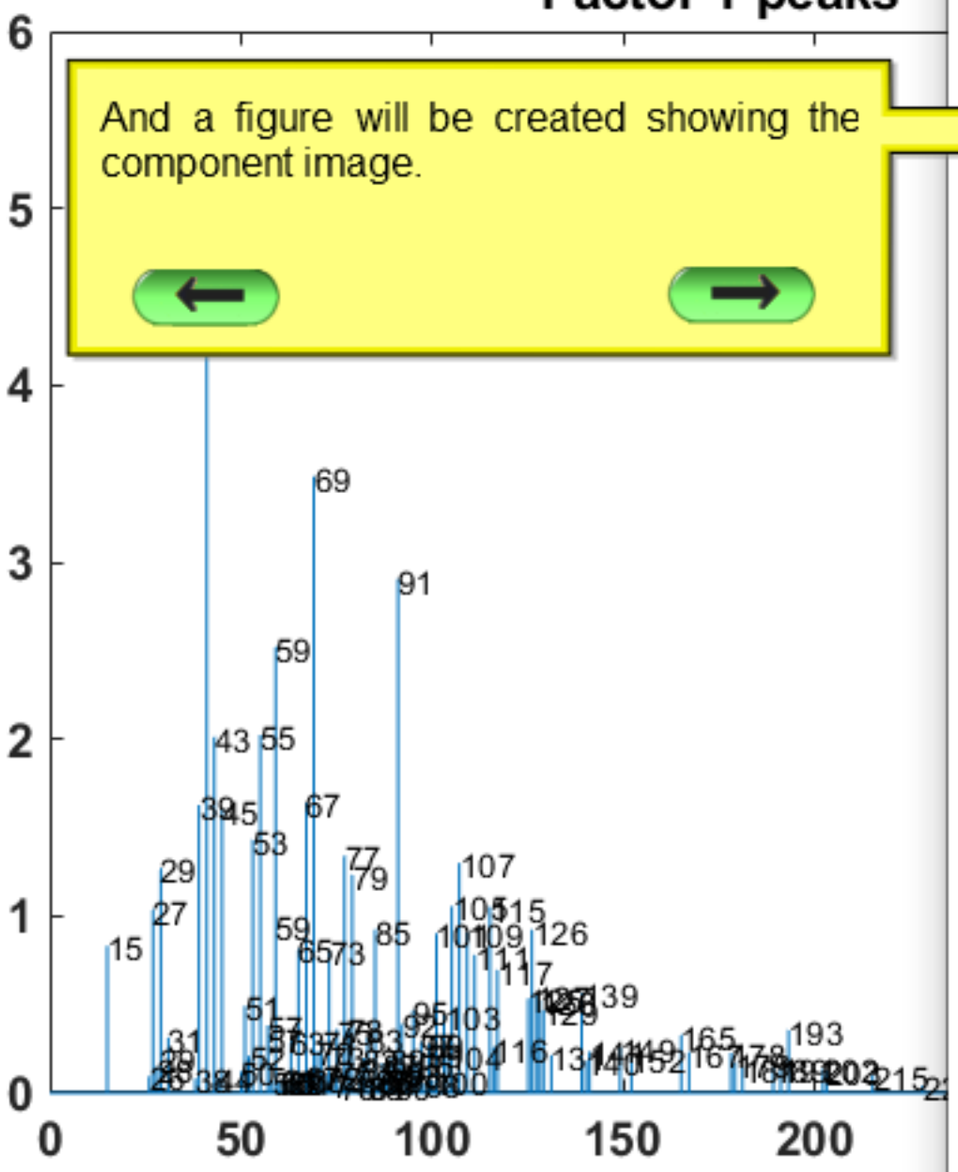
Data Selection Panel

Name of Image Matrix **Name of Variable Matrix**

Figure 6

File Edit View Insert Tools Desktop Window Help

Factor 1 peaks

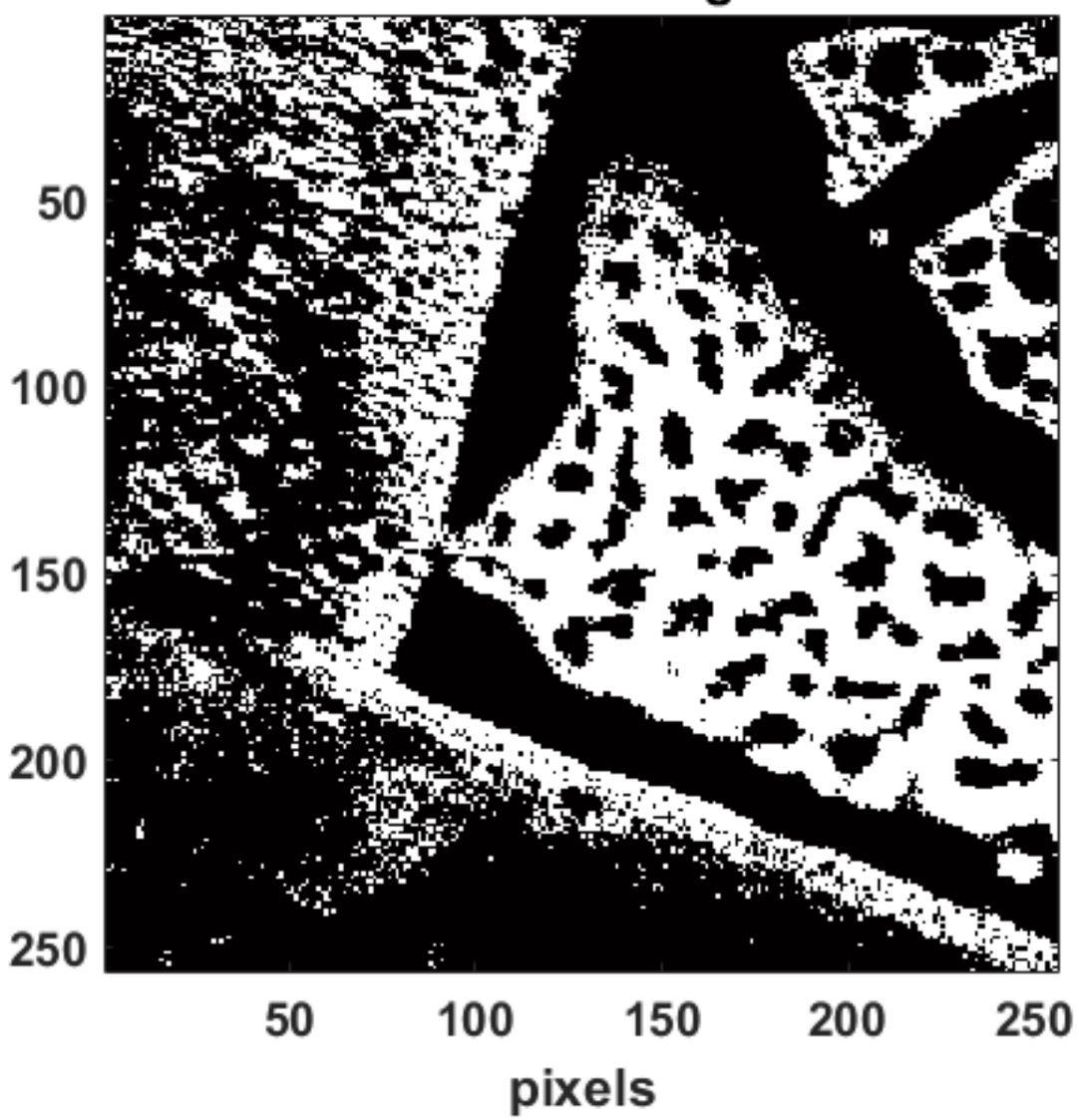


And a figure will be created showing the component image.

Figure 5

File Edit View Insert Tools Desktop Window Help

Factor 1 image



imagegui

File Data Pre Processing MVA Data Display Image Processing

Data Selection Panel

Name of Image Matrix: imagedata_S3_DE...

Name of Variable Matrix: exactmass_S3_DE_...

Load Selected Data

Image: imagedata_S3_DE_03_1

Variables: exactmass_S3_DE_03_1

Choose distance measure: sqeuclidean

Number of factors to calculate: 3

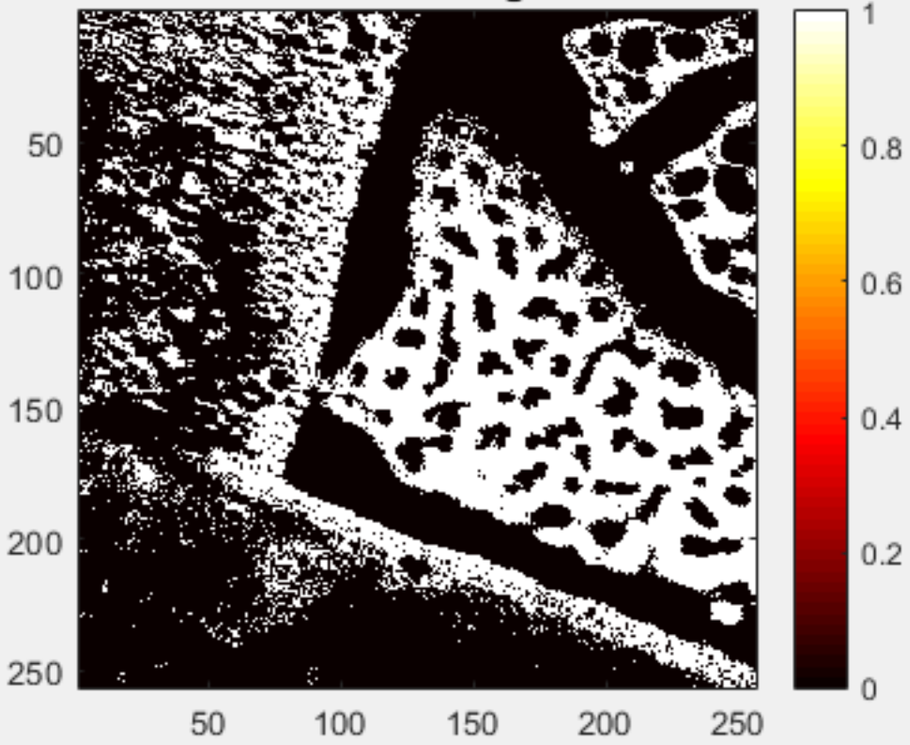
Run K-Means

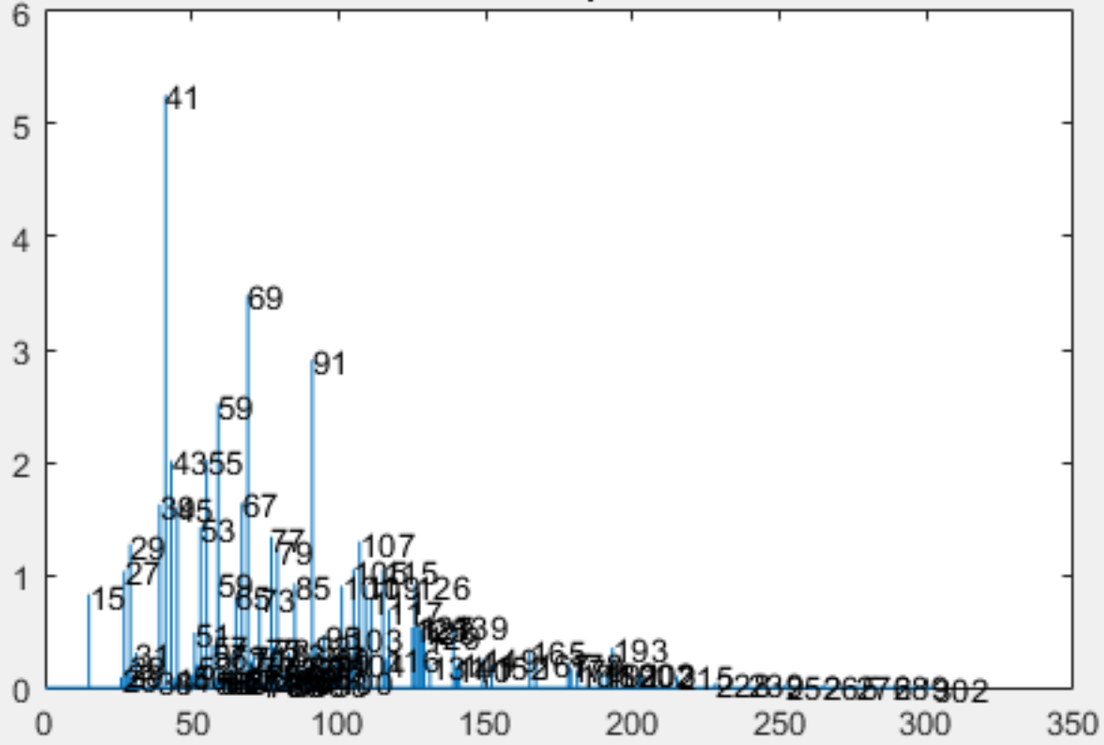
Save K-Means Res..

Press the Save K-Means Res button to save the results for the selected component to ASCII text files.

1

Make Ext





Close panel

imagegui

Save Component Image as

This PC › Documents › MATLAB ›

Search MATLAB

Organize | New folder

- MATLAB
- pngfiles
- SpectraFiles
- Summary
- OneDrive
- This PC
- 3D Objects
- Desktop
- Documents
- Custom Office Templates
- Fax
- MATLAB

Name	Date
A2DP02_Correlation	3/30/2022 10:48 AM
A1DP02_Correlation	3/30/2022 10:45 AM
kmeansSpectra.txt	6/14/2024 2:13 PM
Kmeansresults.txt	6/14/2024 2:13 PM
templist.txt	5/31/2024 2:36 PM
componentspectra.txt	3/15/2024 3:08 PM
Imageidentifiers.txt	3/15/2024 3:08 PM
default2.txt	3/8/2024 3:06 PM
default.txt	3/8/2024 3:05 PM
CH5N2Data.txt	11/10/2022 3:47 PM
Cs2Idata.txt	11/10/2022 3:47 PM
CalcARXPS_Alph0.8.txt	9/1/2022 3:21 PM

File name: KmeansImage.txt

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

Hide Folders

Save | Cancel

A dialog box will open asking for the name for the image data.

-Means

Means Res...

Ext

Close panel

imagegui

Save Component Spectra as

This PC › Documents › MATLAB ›

Search MATLAB

Organize New folder

MATLAB
pngfiles
SpectraFiles
Summary
OneDrive
This PC
3D Objects
Desktop
Documents
Custom Office Templates
Fax
MATLAB

Name	Date
A2DP02_Correlation	3/30/2022 10:48 AM
A1DP02_Correlation	3/30/2022 10:45 AM
KmeansImage.txt	6/14/2024 2:14 PM
kmeansSpectra.txt	6/14/2024 2:13 PM
Kmeansresults.txt	6/14/2024 2:13 PM
templist.txt	5/31/2024 2:36 PM
componentspectra.txt	3/15/2024 3:08 PM
Imageidentifiers.txt	3/15/2024 3:08 PM
default2.txt	3/8/2024 3:06 PM
default.txt	3/8/2024 3:05 PM
CH5N2Data.txt	11/10/2022 3:47 PM
Cs2Idata.txt	11/10/2022 3:47 PM

File name: KmeansSpectra.txt

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

Hide Folders

Save Cancel

And then a dialogue box will open asking for a name for the component spectrum.

-Means

Means Res...

Ext

Close panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

Data Selection Panel

Name of Image Matrix: imagedata_S3_DE...

Name of Variable Matrix: exactmass_S3_DE_...

Load Selected Data

Image: imagedata_S3_DE_03_1

Variables: exactmass_S3_DE_03_1

Choose distance measure: sqeuclidean

Choose cluster measure: cluster

Number of factors to calculate: 3

Number of iterations: 5

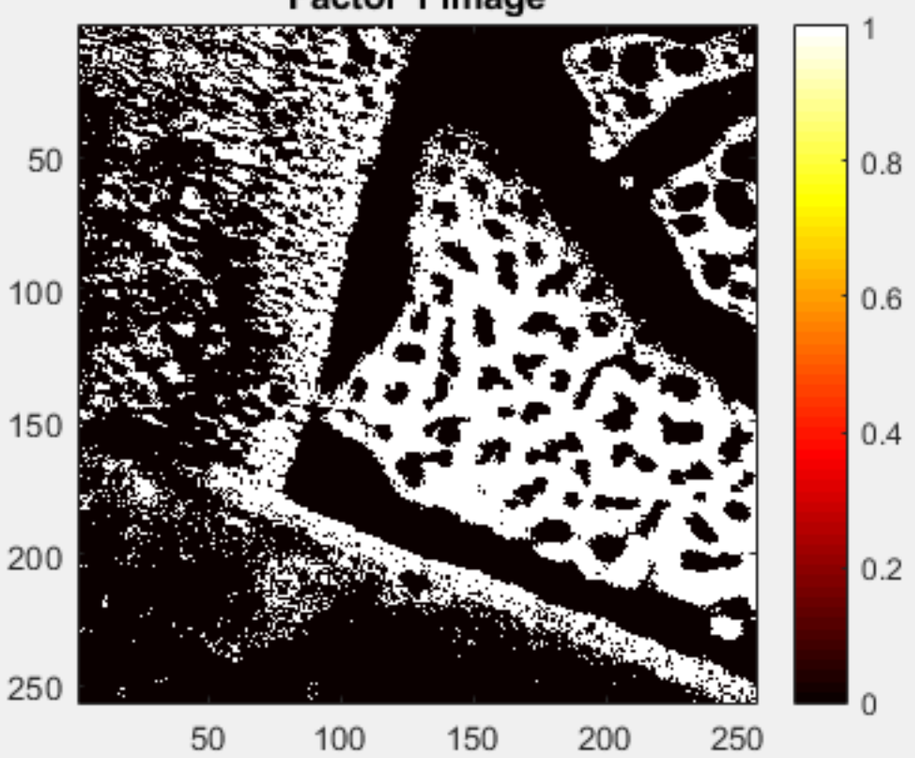
Run K-Means

Save K-Means Res..

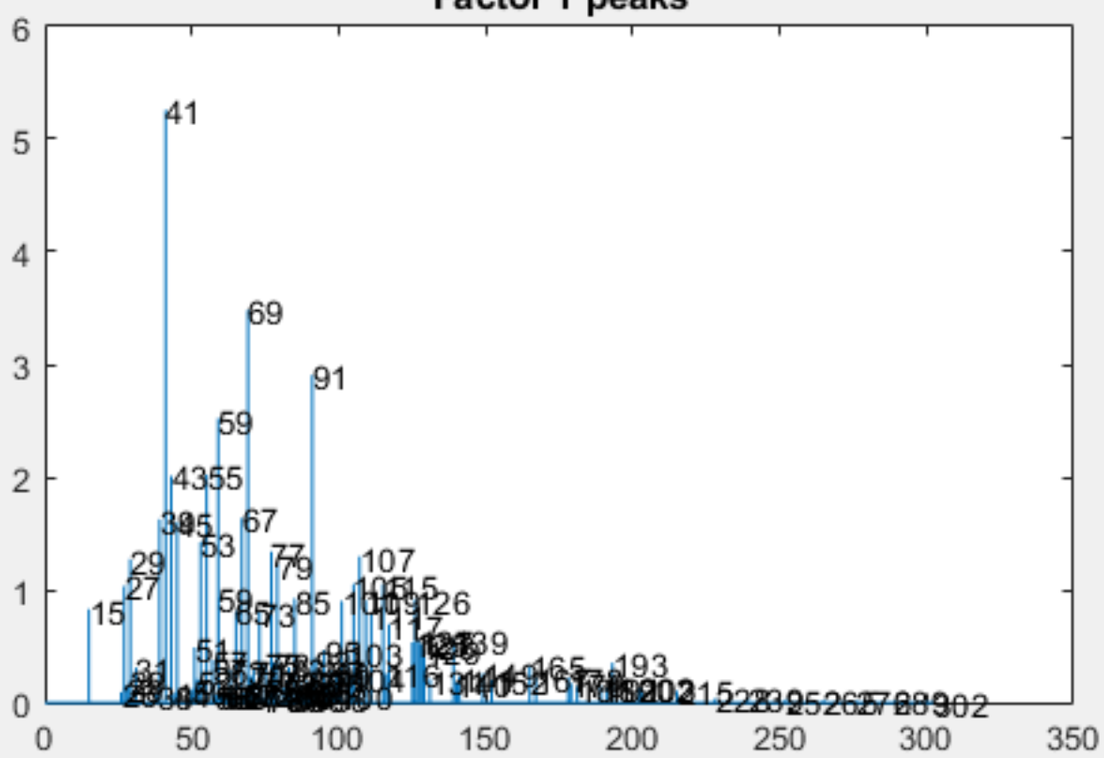
1

Plot Sel Comp Plot All Comp Save Fig Make Ext

Factor 1 image



Factor 1 peaks



Press the Close Panel button close and reset the K-means panel.

Close panel

imagegui

File Data Pre Processing MVA Data Display Image Processing

Data Selection Panel

Name of Image Matrix imagedata_S3_DE...

Name of Variable Matrix exactmass_S3_DE_...

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 tutorials for detailed information on how to use each function in the imagegui.