

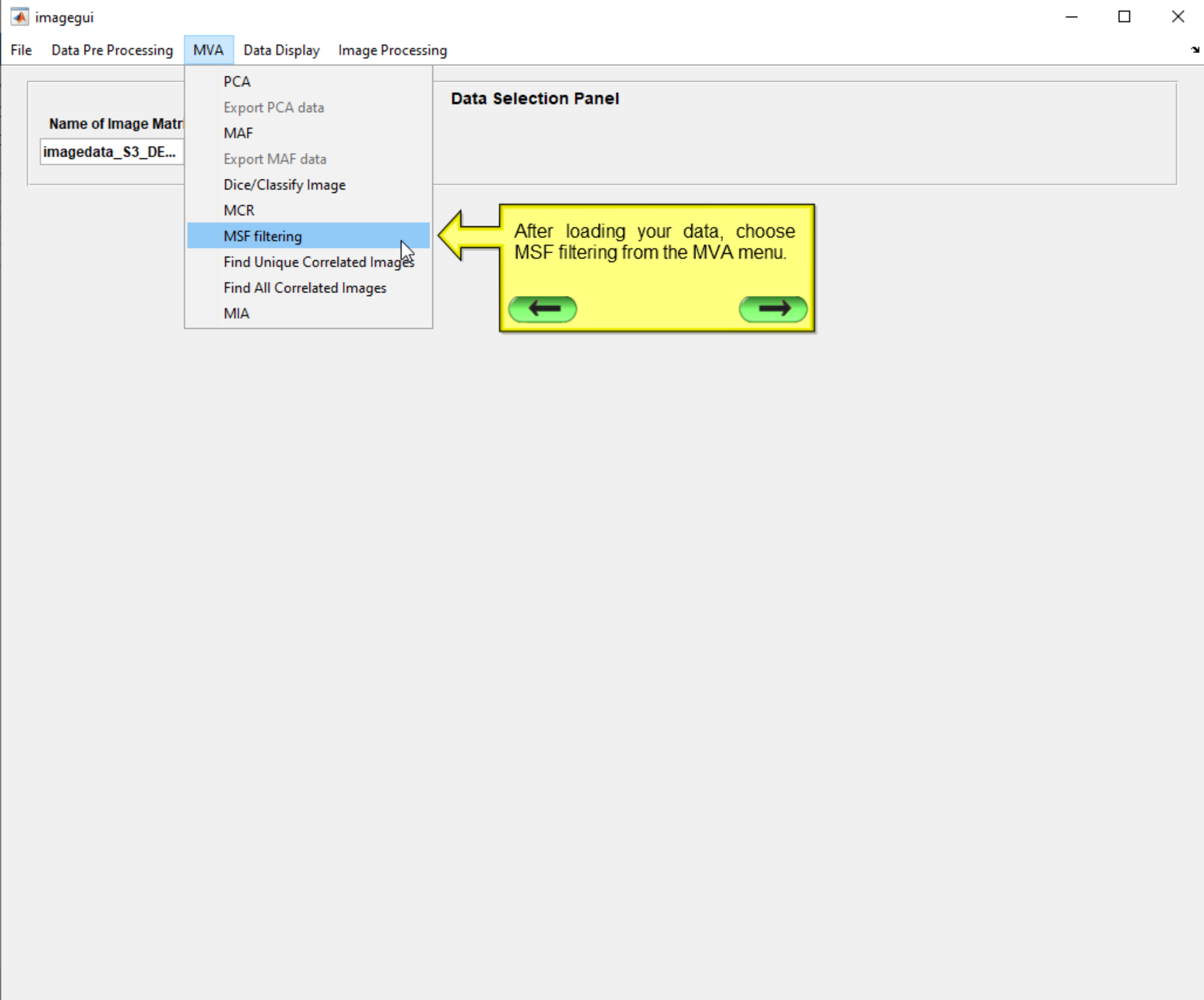
This tutorial covers how to use the MFS filtering functions discussed in the paper:

Tyler et. al., "Denoising of Mass Spectrometry Images via Inverse Maximum Signal Factors Analysis", Anal. Chem. 2022, 94, 2835–2843.

The functions were written by Professor Bonnie Tyler and adapted into the NBToolbox with permission.

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.





Name of Image Matrix

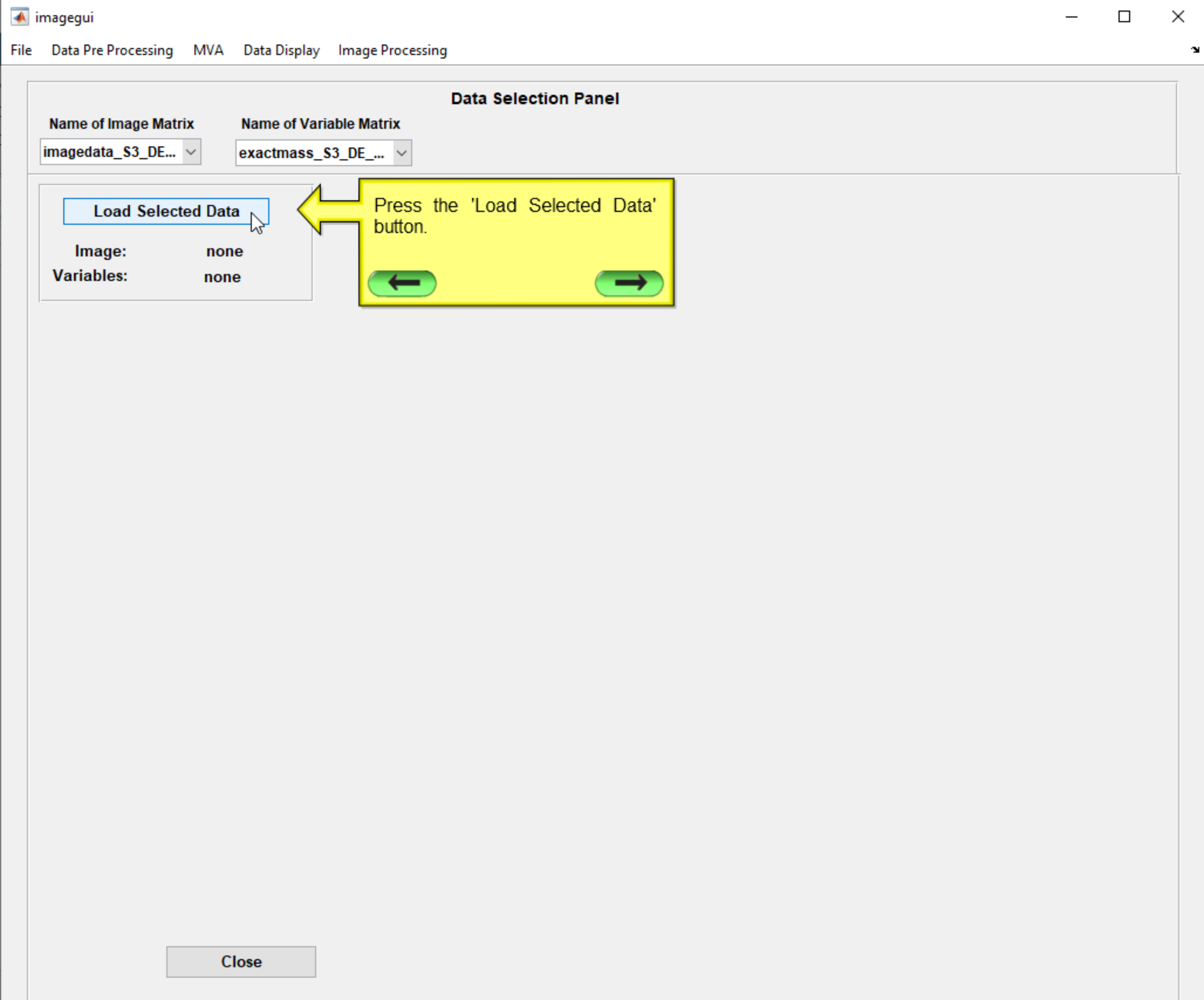
imagedata_S3_DE...

- PCA
- Export PCA data
- MAF
- Export MAF data
- Dice/Classify Image
- MCR
- MSF filtering**
- Find Unique Correlated Images
- Find All Correlated Images
- MIA

Data Selection Panel

After loading your data, choose MSF filtering from the MVA menu.





Data Selection Panel

Name of Image Matrix

Name of Variable Matrix

imagedata_S3_DE...

exactmass_S3_DE...

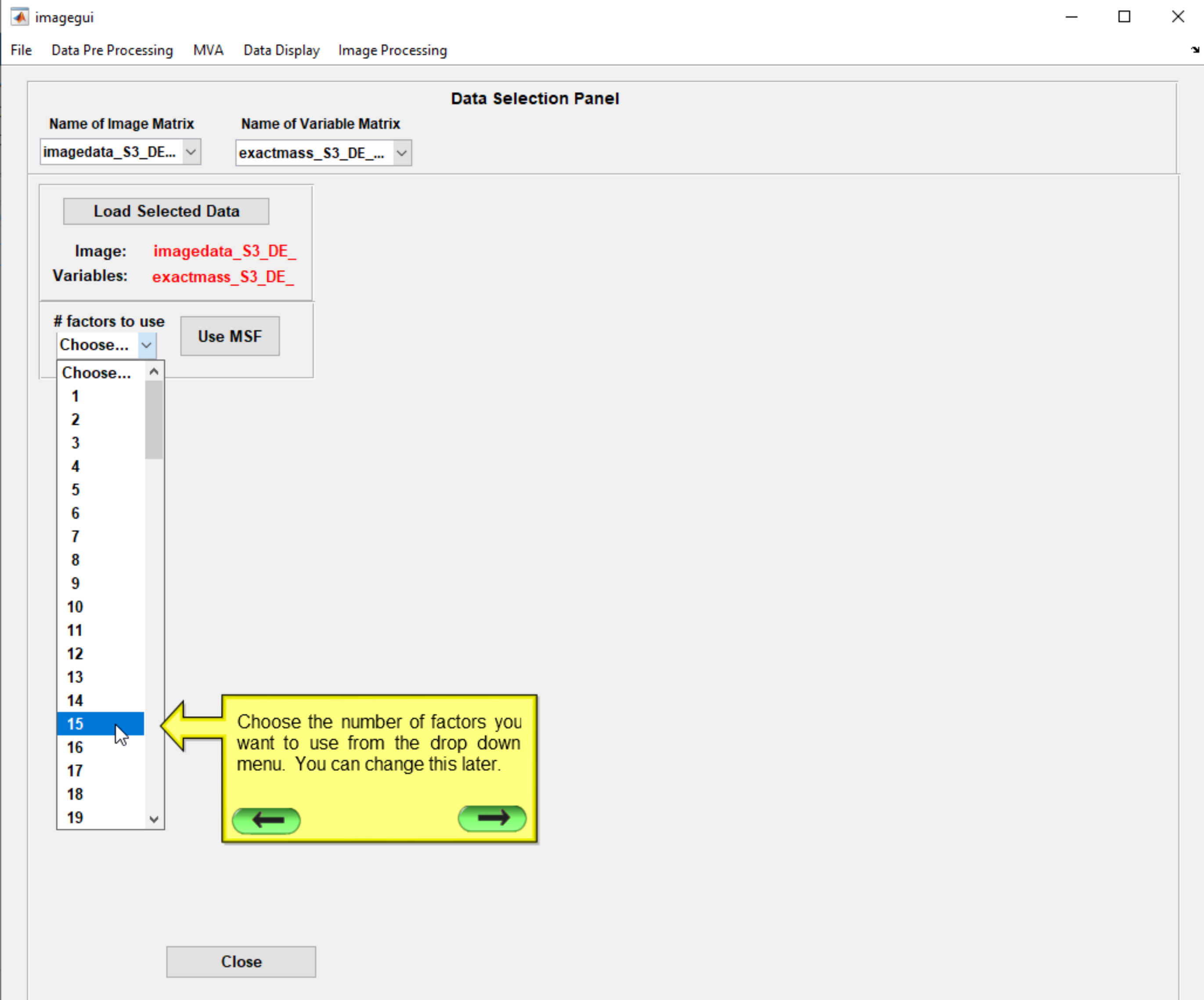
Load Selected Data

Press the 'Load Selected Data' button.



Image: none
Variables: none

Close



Data Selection Panel

Name of Image Matrix

imagedata_S3_DE...

Name of Variable Matrix

exactmass_S3_DE...

Load Selected Data

Image: imagedata_S3_DE_

Variables: exactmass_S3_DE_

factors to use

Choose...

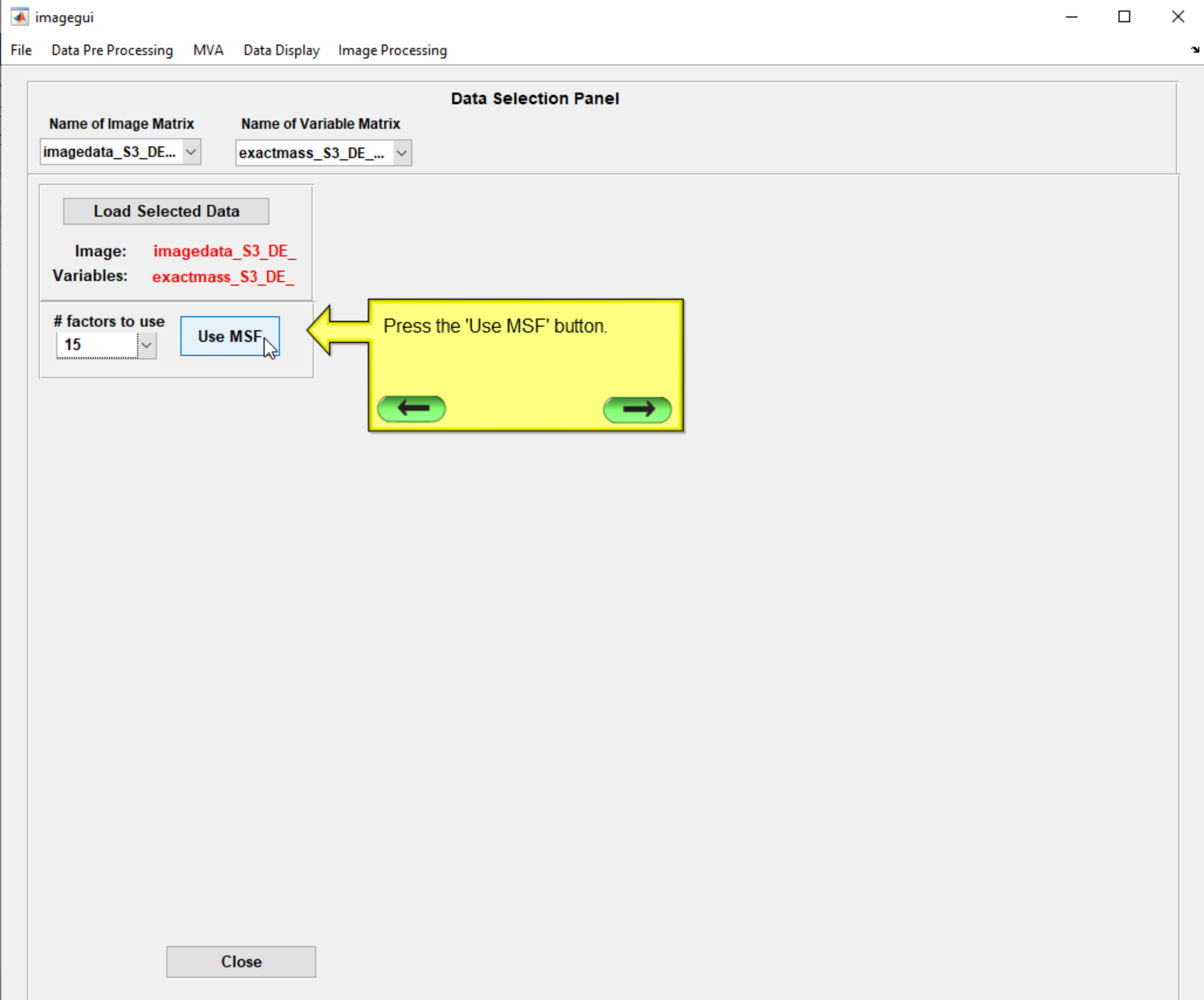
Use MSF

Choose...

- 1
- 2
- 3
- 4
- 5
- 6
- 7
- 8
- 9
- 10
- 11
- 12
- 13
- 14
- 15
- 16
- 17
- 18
- 19

Choose the number of factors you want to use from the drop down menu. You can change this later.

Close



Data Selection Panel

Name of Image Matrix

imagedata_S3_DE...

Name of Variable Matrix

exactmass_S3_DE...

Load Selected Data

Image: imagedata_S3_DE_
Variables: exactmass_S3_DE_

factors to use

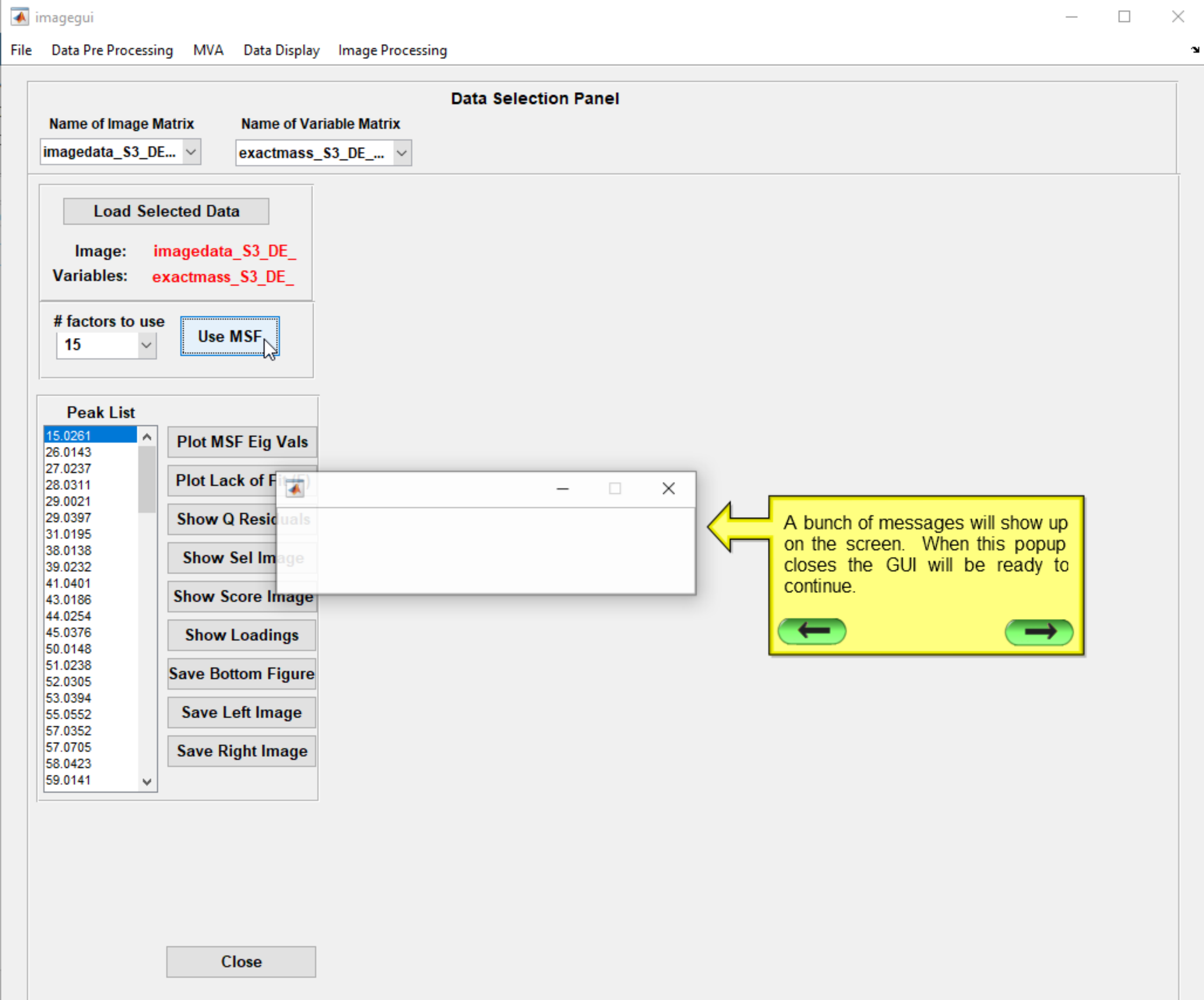
15

Use MSF

Press the 'Use MSF' button.



Close



Data Selection Panel

Name of Image Matrix

imagedata_S3_DE...

Name of Variable Matrix

exactmass_S3_DE...

Load Selected Data

Image: imagedata_S3_DE_

Variables: exactmass_S3_DE_

factors to use

15

Use MSF

Peak List

15.0261

26.0143

27.0237

28.0311

29.0021

29.0397

31.0195

38.0138

39.0232

41.0401

43.0186

44.0254

45.0376

50.0148

51.0238

52.0305

53.0394

55.0552

57.0352

57.0705

58.0423

59.0141

Plot MSF Eig Vals

Plot Lack of Fit

Show Q Residuals

Show Sel Image

Show Score Image

Show Loadings

Save Bottom Figure

Save Left Image

Save Right Image

Close

A bunch of messages will show up on the screen. When this popup closes the GUI will be ready to continue.

Data Selection Panel

Name of Image Matrix

imagedata_S3_DE...

Name of Variable Matrix

exactmass_S3_DE...

Load Selected Data

Image: imagedata_S3_DE_

Variables: exactmass_S3_DE_

factors to use

15

Use MSF

Peak List

15.0261
26.0143
27.0237
28.0311
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31.0195
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39.0232
41.0401
43.0186
44.0254
45.0376
50.0148
51.0238
52.0305
53.0394
55.0552
57.0352
57.0705
58.0423
59.0141

Plot MSF Eig Vals

Plot Lack of Fit (F)

Show Q Residuals

Show Sel Image

Show Score Image

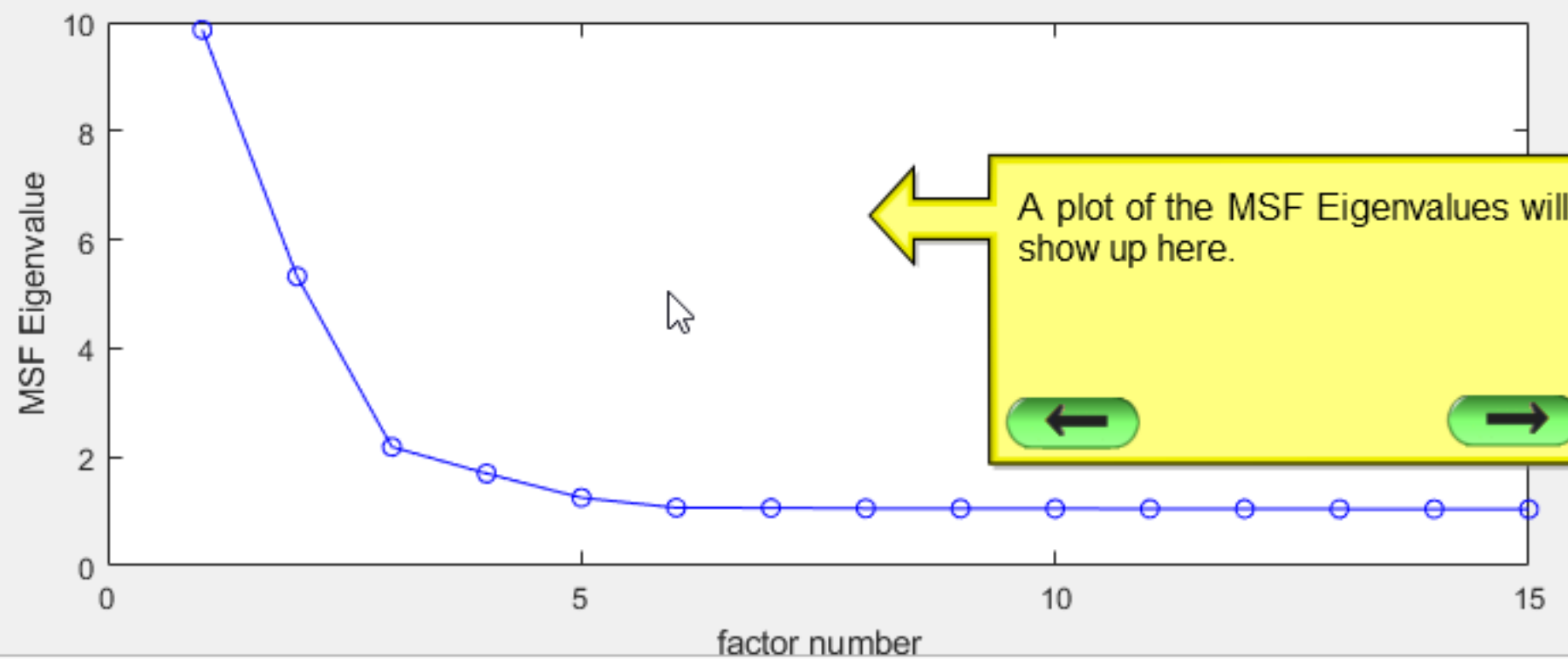
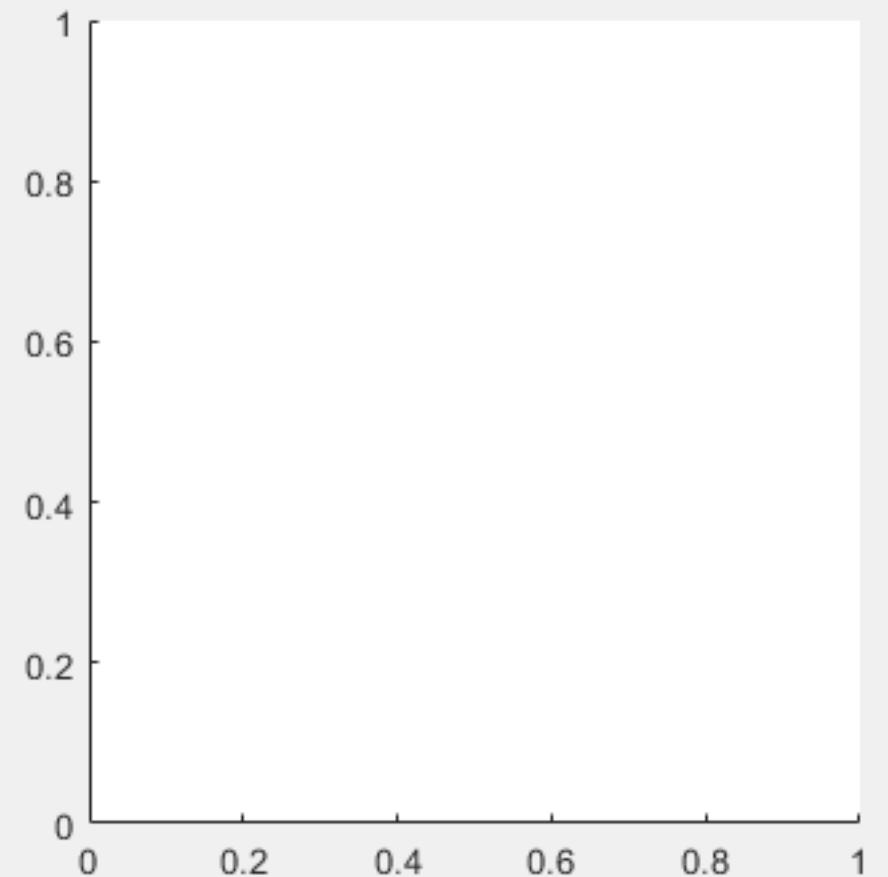
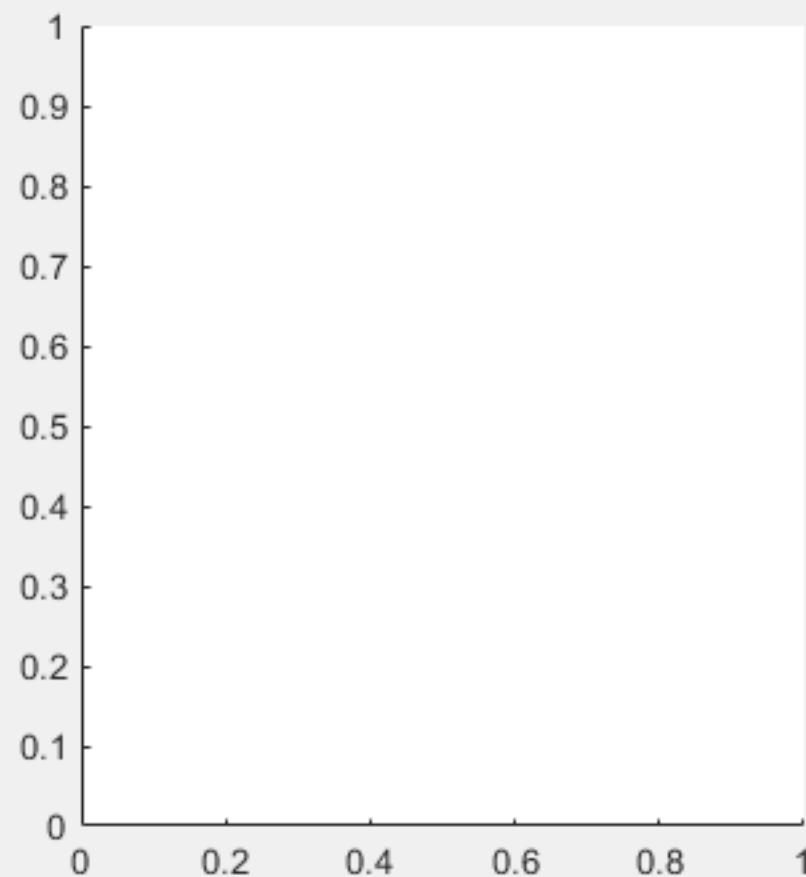
Show Loadings

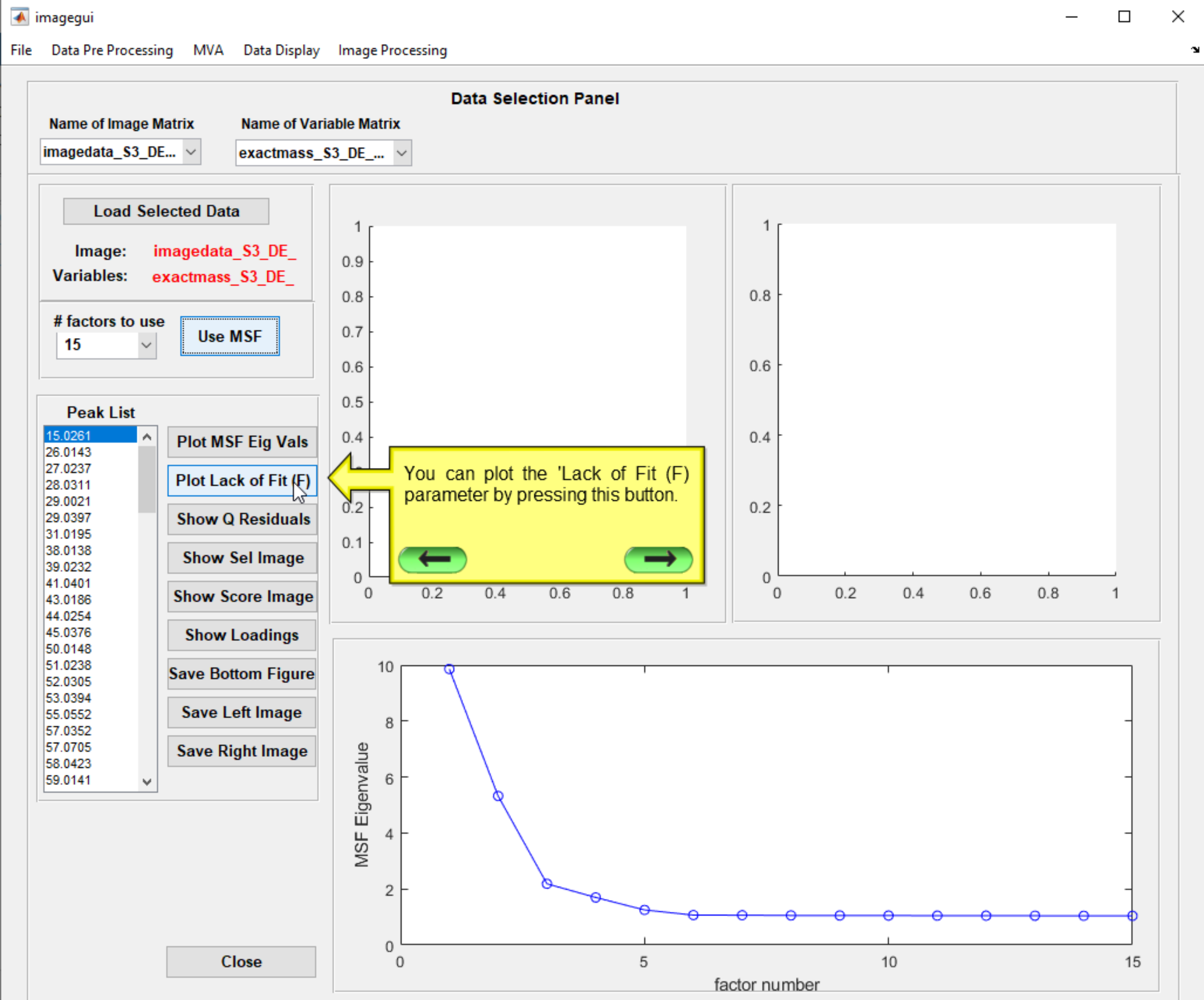
Save Bottom Figure

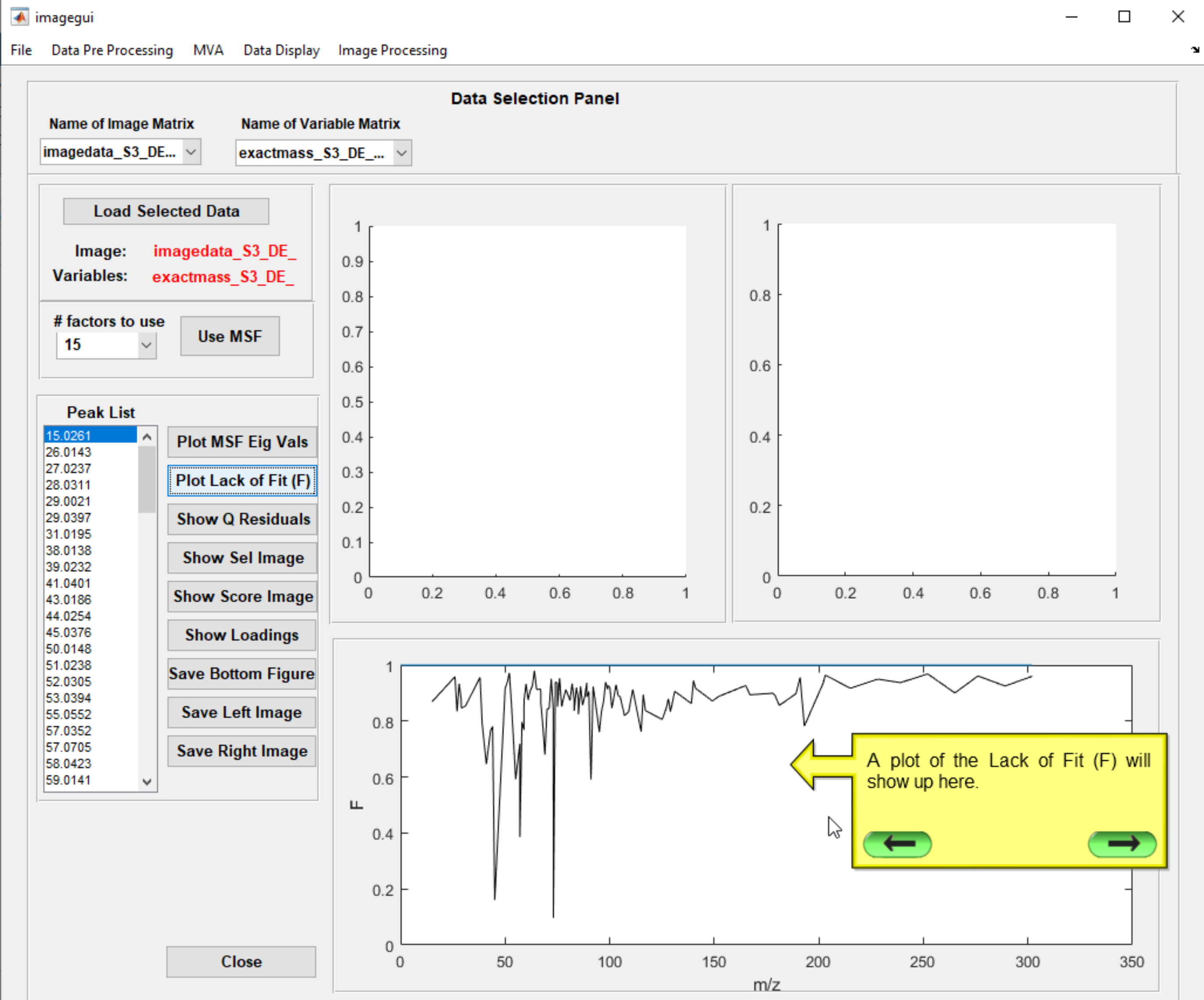
Save Left Image

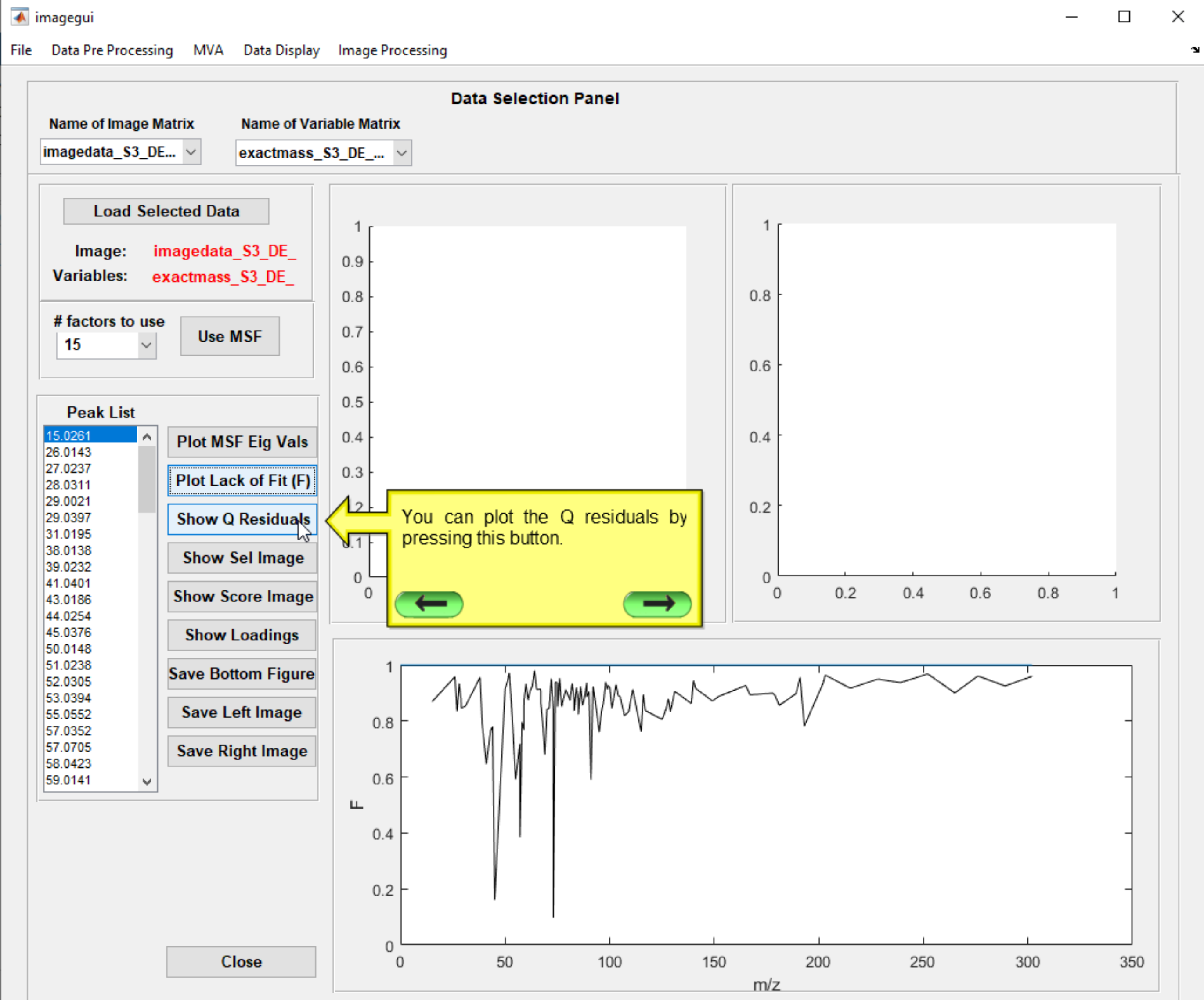
Save Right Image

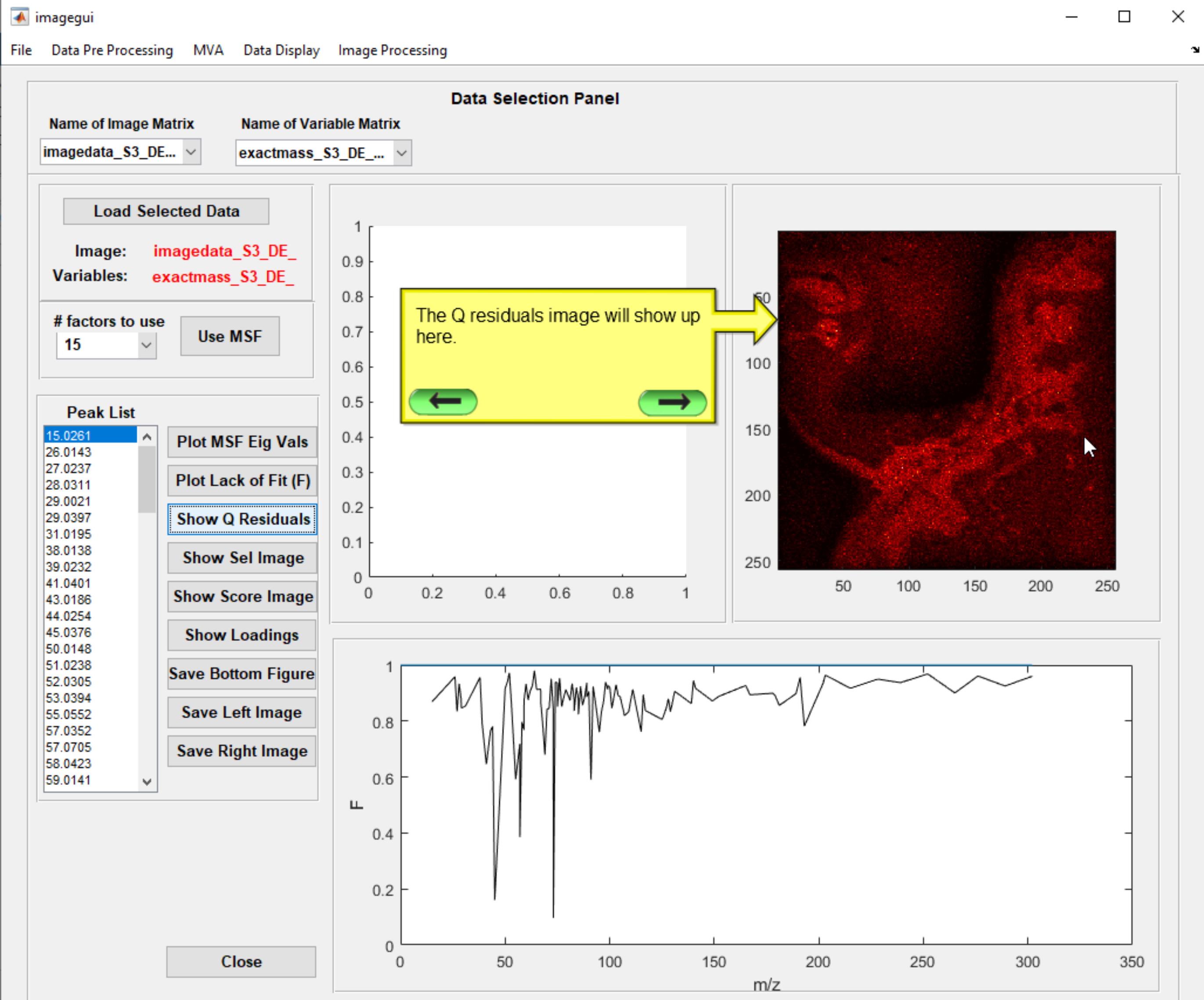
Close

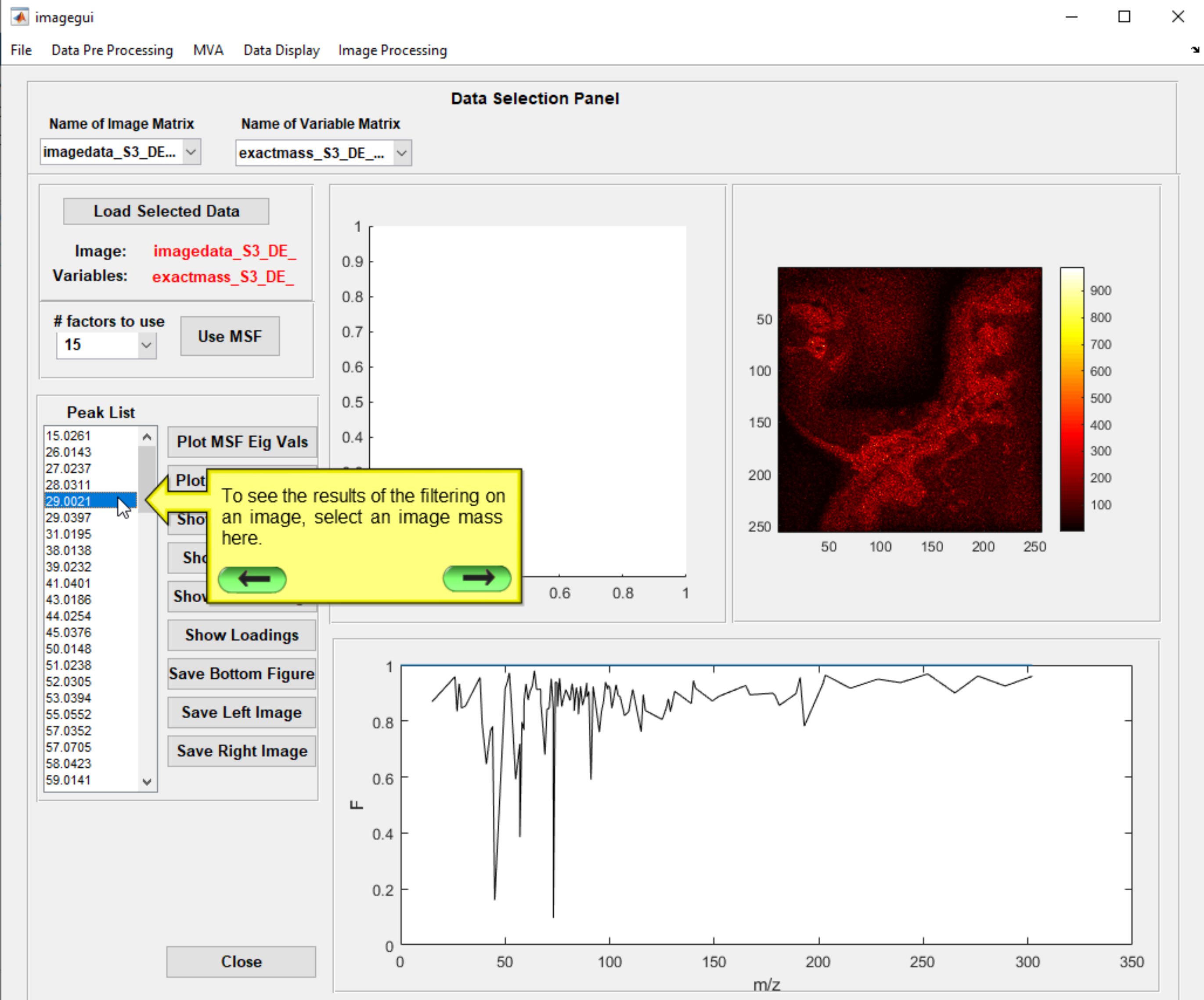


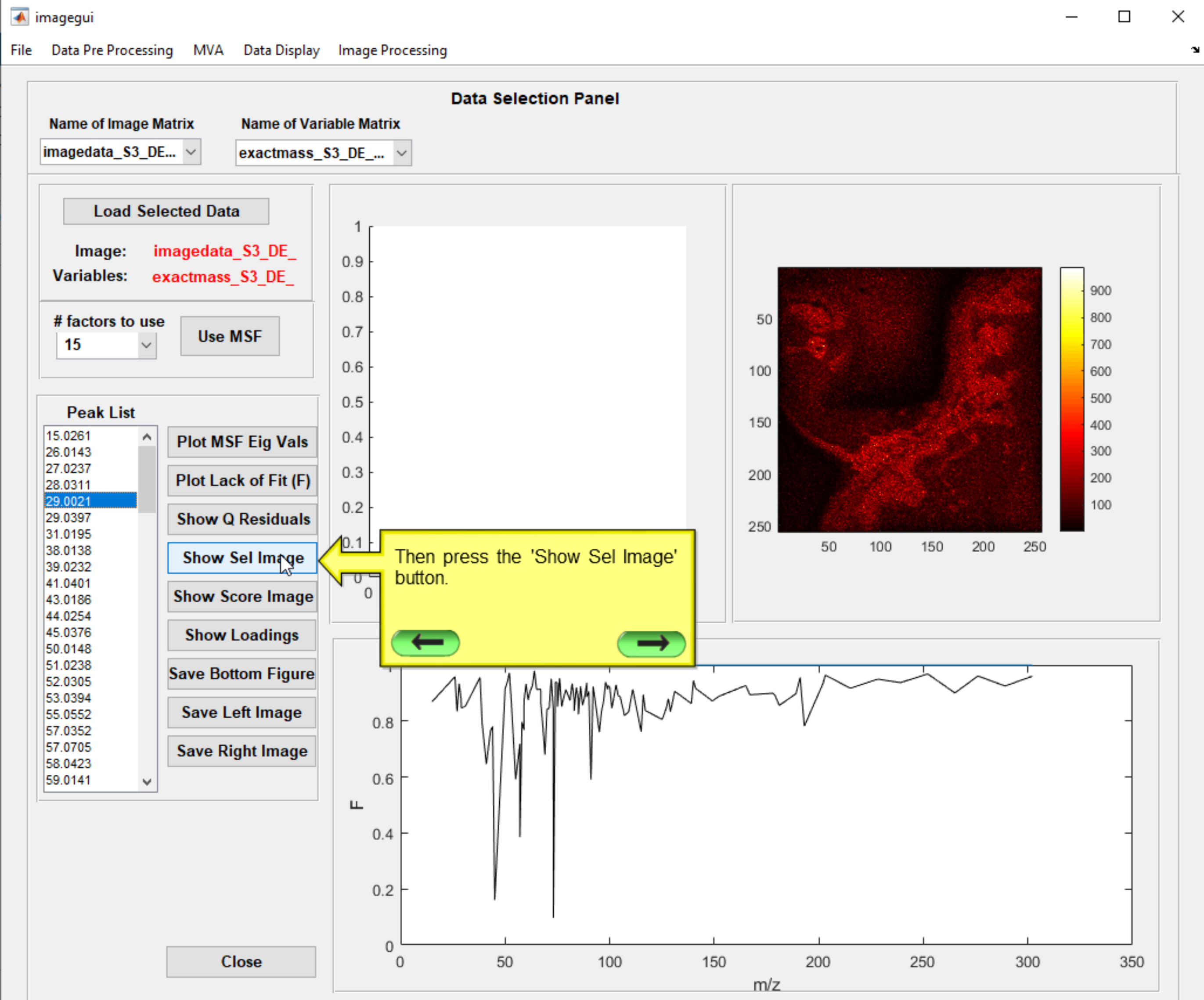












Data Selection Panel

Name of Image Matrix

imagedata_S3_DE...

Name of Variable Matrix

exactmass_S3_DE...

Load Selected Data

Image: imagedata_S3_DE_

Variables: exactmass_S3_DE_

The original image and filtered images will show up in these plots.



26.0143
27.0237
28.0311
29.0021
29.0397
31.0195
38.0138
39.0232
41.0401
43.0186
44.0254
45.0376
50.0148
51.0238
52.0305
53.0394
55.0552
57.0352
57.0705
58.0423
59.0141

Plot Lack of Fit (F)

Show Q Residuals

Show Sel Image

Show Score Image

Show Loadings

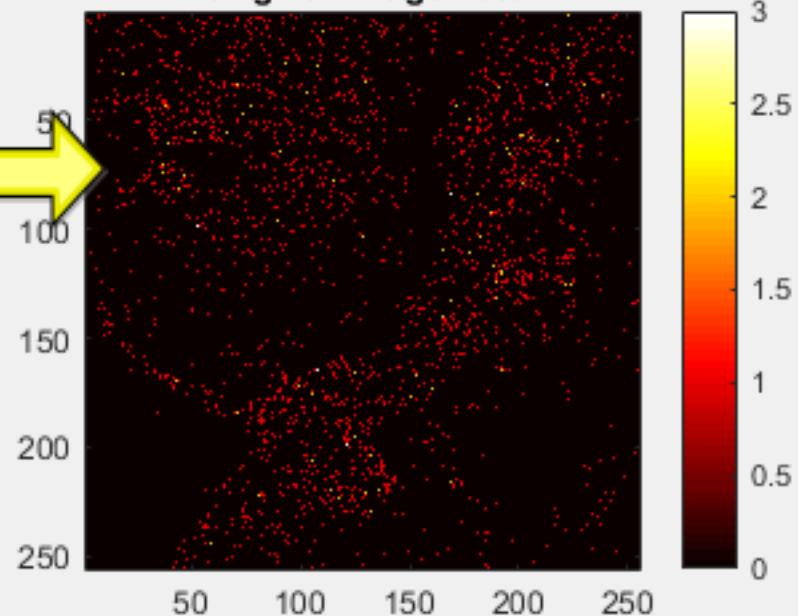
Save Bottom Figure

Save Left Image

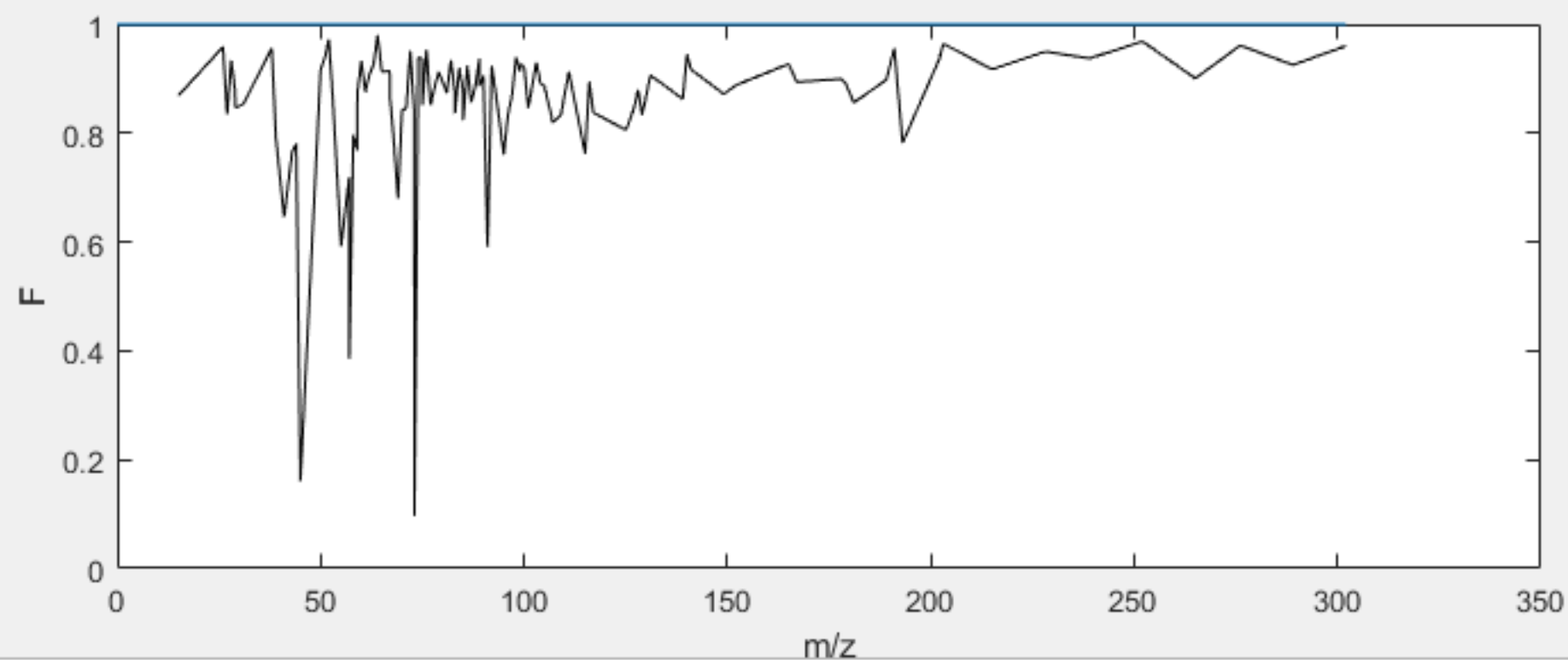
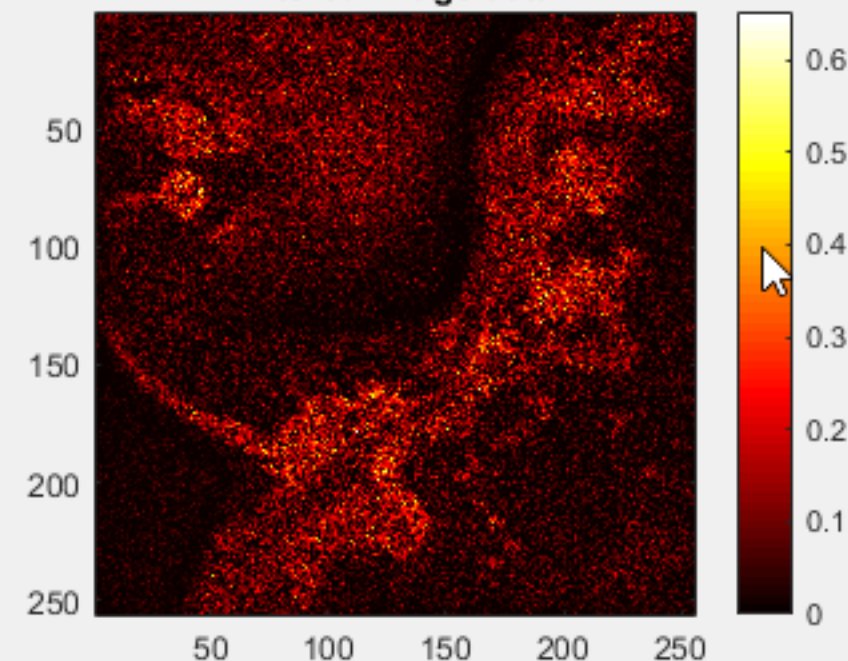
Save Right Image

Close

Original image data



Filtered image data



Data Selection Panel

Name of Image Matrix

imagedata_S3_DE...

Name of Variable Matrix

exactmass_S3_DE...

Load Selected Data

Image: imagedata_S3_DE_

Variables: exactmass_S3_DE_

factors to use

15

Use MSF

Peak List

15.0261
26.0143
27.0237
28.0311
29.0021
29.0397
31.0195
38.0138
39.0232
41.0401
43.0186
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45.0376
50.0148
51.0238
52.0305
53.0394
55.0552
57.0352
57.0705
58.0423
59.0141

Plot MSF Eig Vals

Plot Lack of Fit (F)

Show Q Residuals

Show Sel Image

Show Score Image

Show Loadings

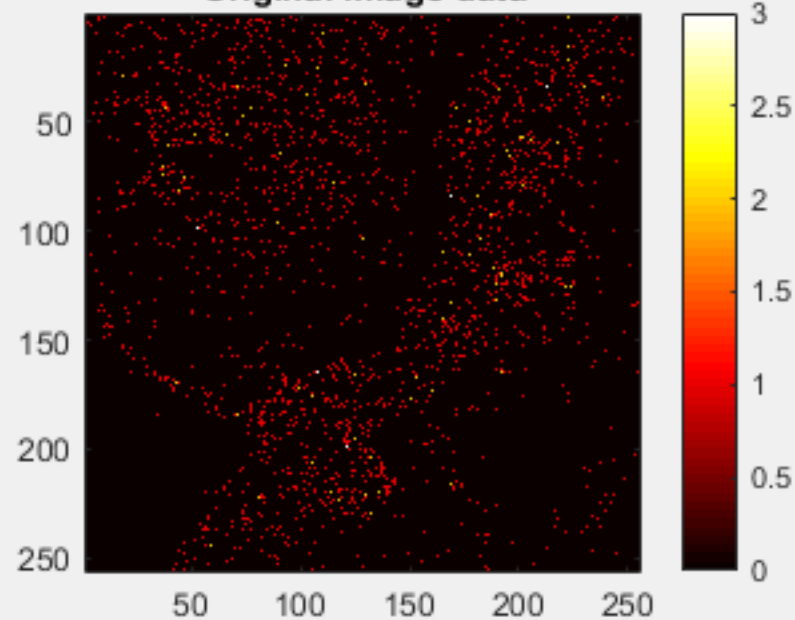
Save Bottom Figure

Save Left Image

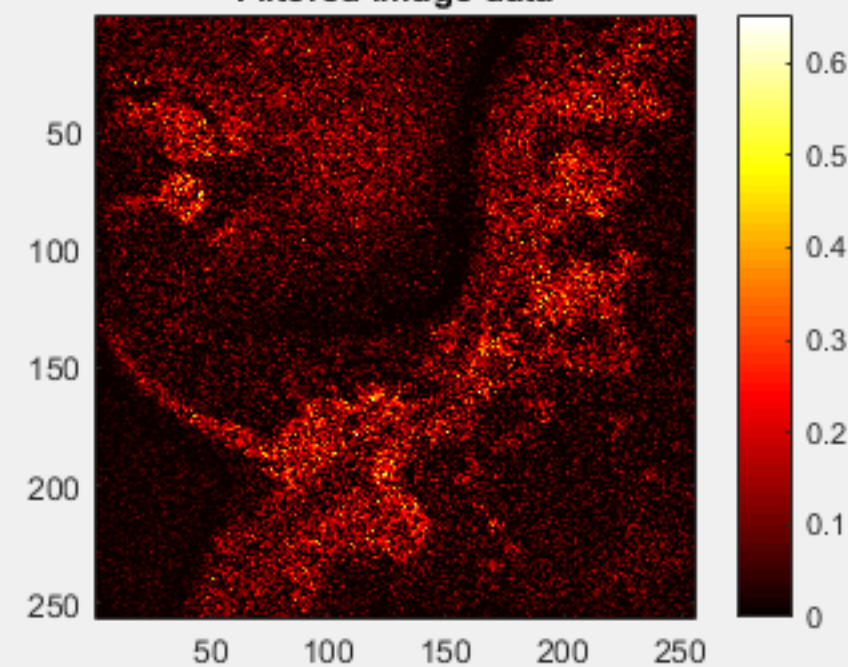
Save Right Image

Close

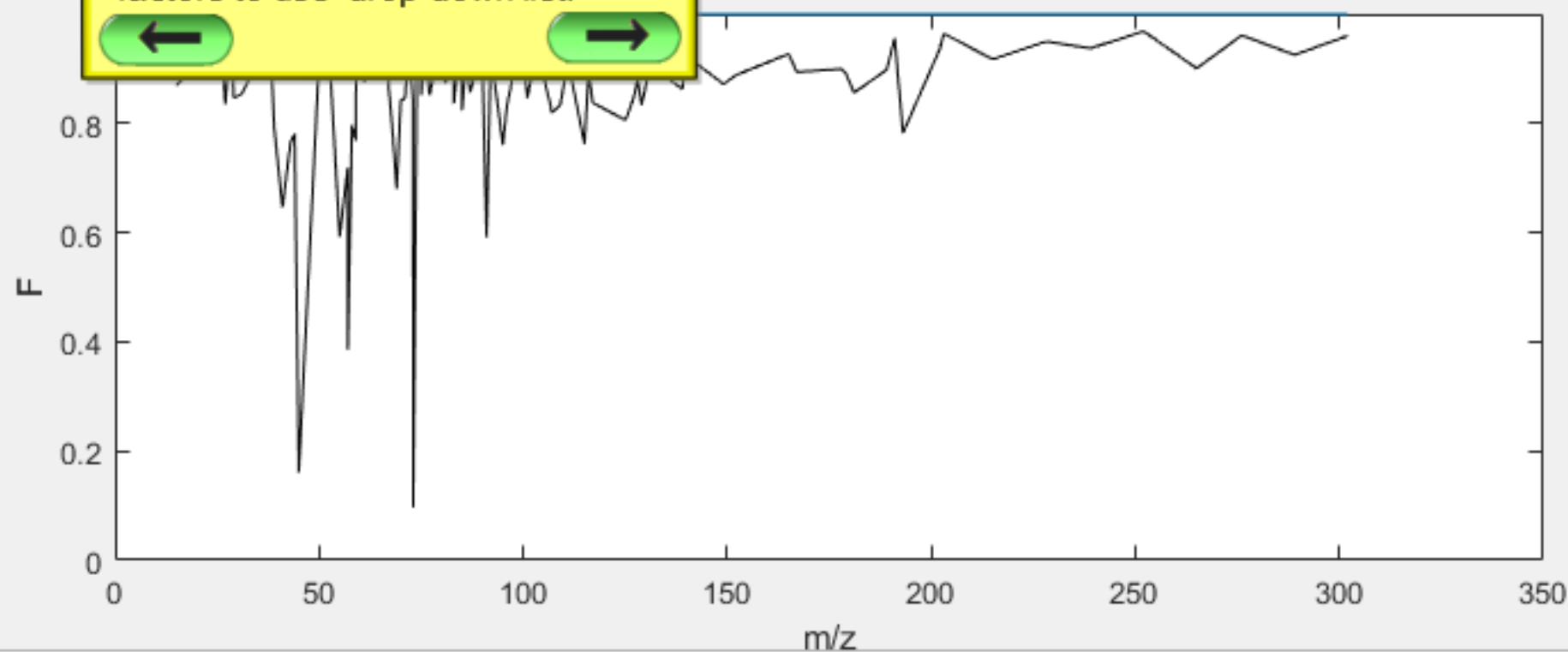
Original image data



Filtered image data



Press the 'Show Score Image' button to display the scores for the selected factor number from the 'factors to use' drop down list.



Data Selection Panel

Name of Image Matrix

imagedata_S3_DE...

Name of Variable Matrix

exactmass_S3_DE...

Load Selected Data

Image: imagedata_S3_DE_

Variables: exactmass_S3_DE_

factors to use

15

Use MSF

Peak List

15.0261
26.0143
27.0237
28.0311
29.0021
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31.0195
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39.0232
41.0401
43.0186
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45.0376
50.0148
51.0238
52.0305
53.0394
55.0552
57.0352
57.0705
58.0423
59.0141

Plot MSF Eig Vals

Plot Lack of Fit (F)

Show Q Residuals

Show Sel Image

Show Score Image

Show Loadings

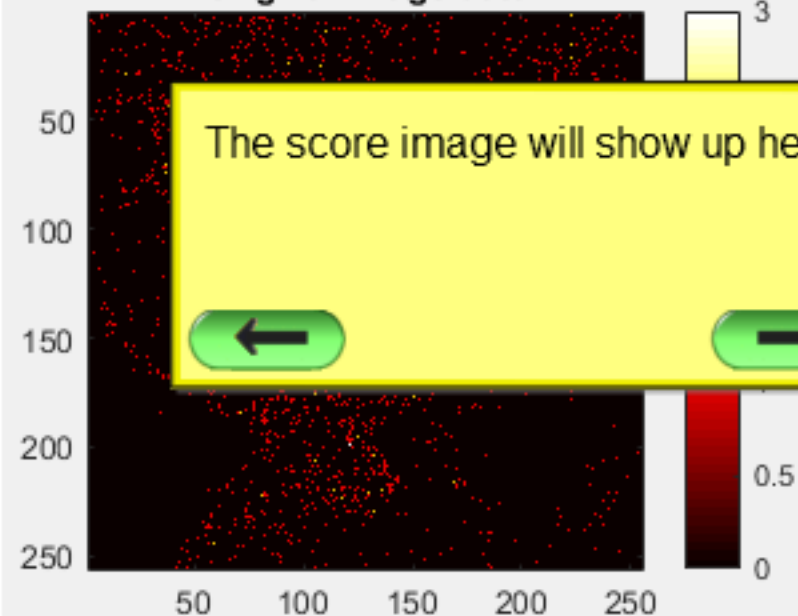
Save Bottom Figure

Save Left Image

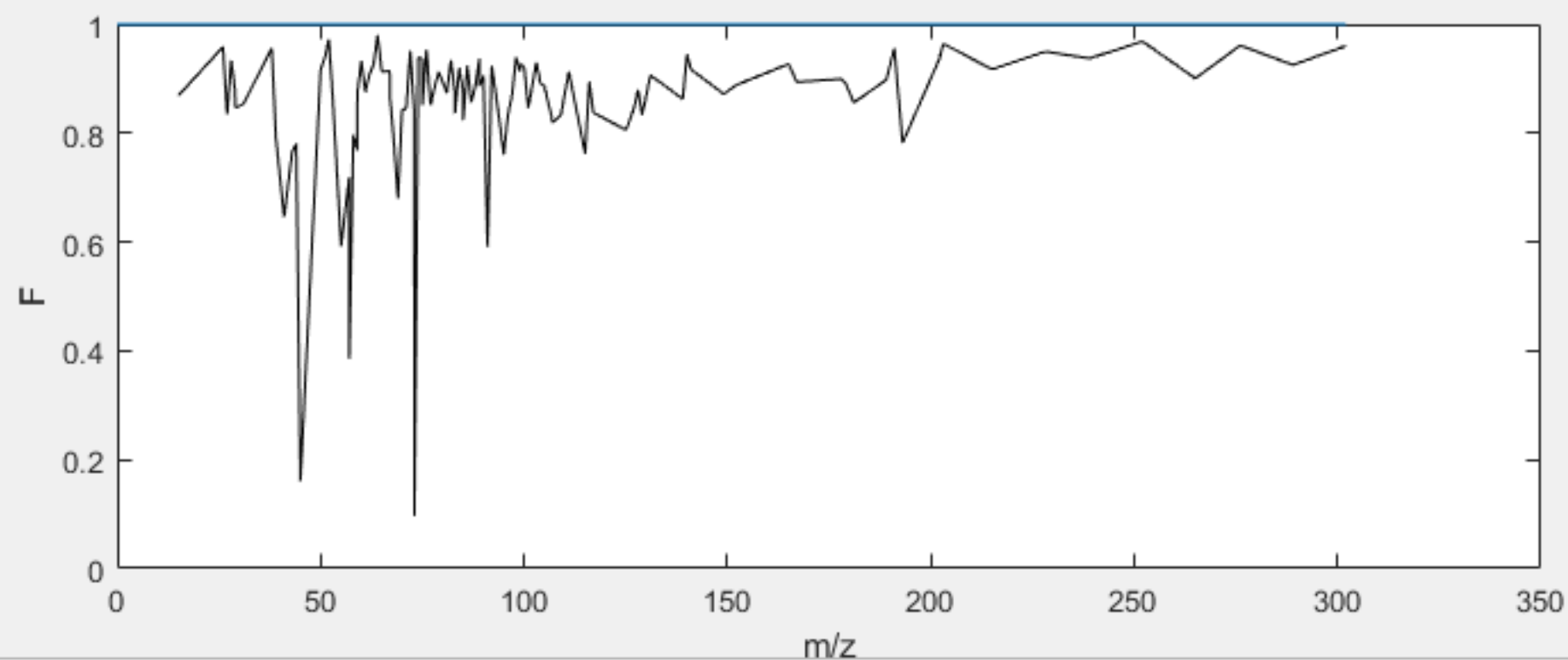
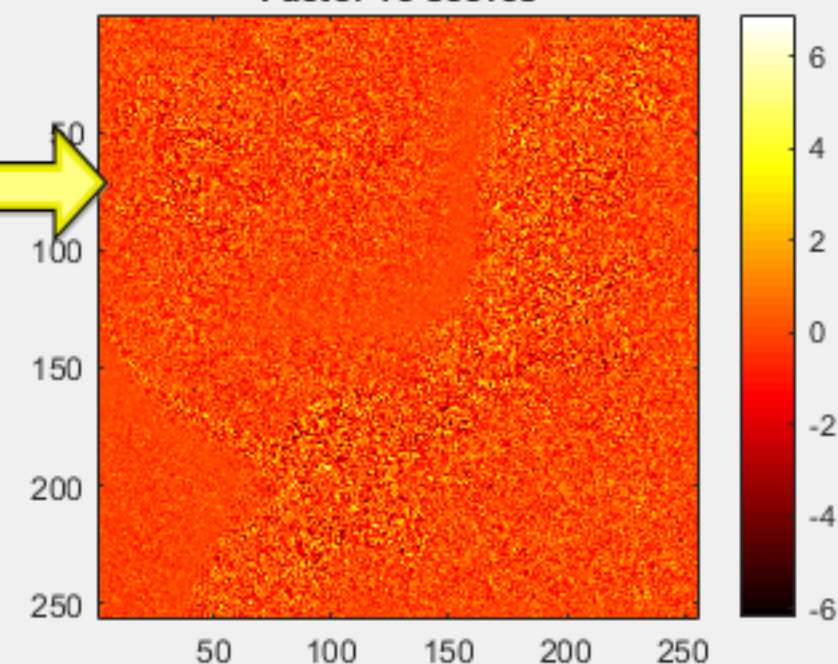
Save Right Image

Close

Original image data



Factor 15 scores



Data Selection Panel

Name of Image Matrix

imagedata_S3_DE...

Name of Variable Matrix

exactmass_S3_DE...

Load Selected Data

Image: imagedata_S3_DE_

Variables: exactmass_S3_DE_

factors to use

15

Use MSF

Peak List

15.0261
26.0143
27.0237
28.0311
29.0021
29.0397
31.0195
38.0138
39.0232
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44.0254
45.0376
50.0148
51.0238
52.0305
53.0394
55.0552
57.0352
57.0705
58.0423
59.0141

Plot MSF Eig Vals

Plot Lack of Fit (F)

Show Q Residuals

Show Sel Image

Show Score Image

Show Loadings

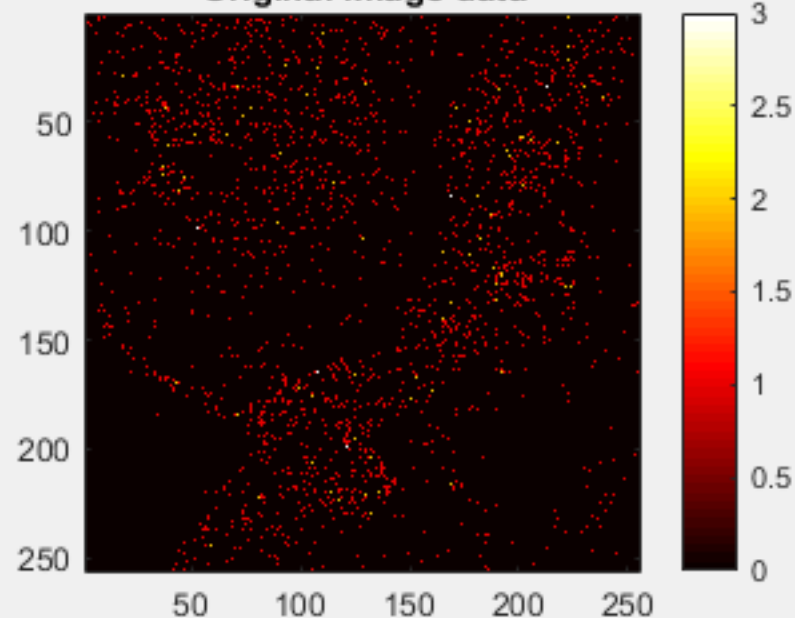
Save Bottom Figure

Save Left Image

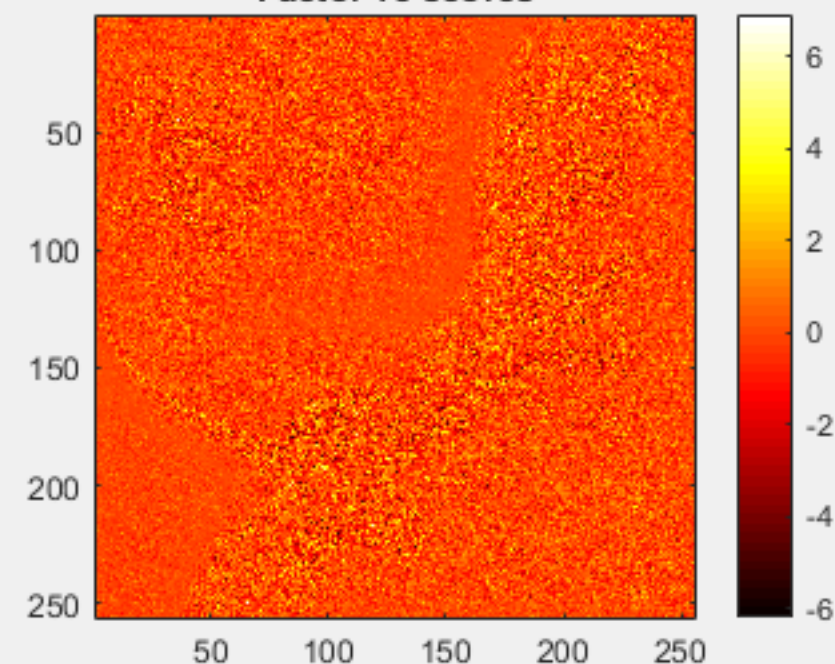
Save Right Image

Close

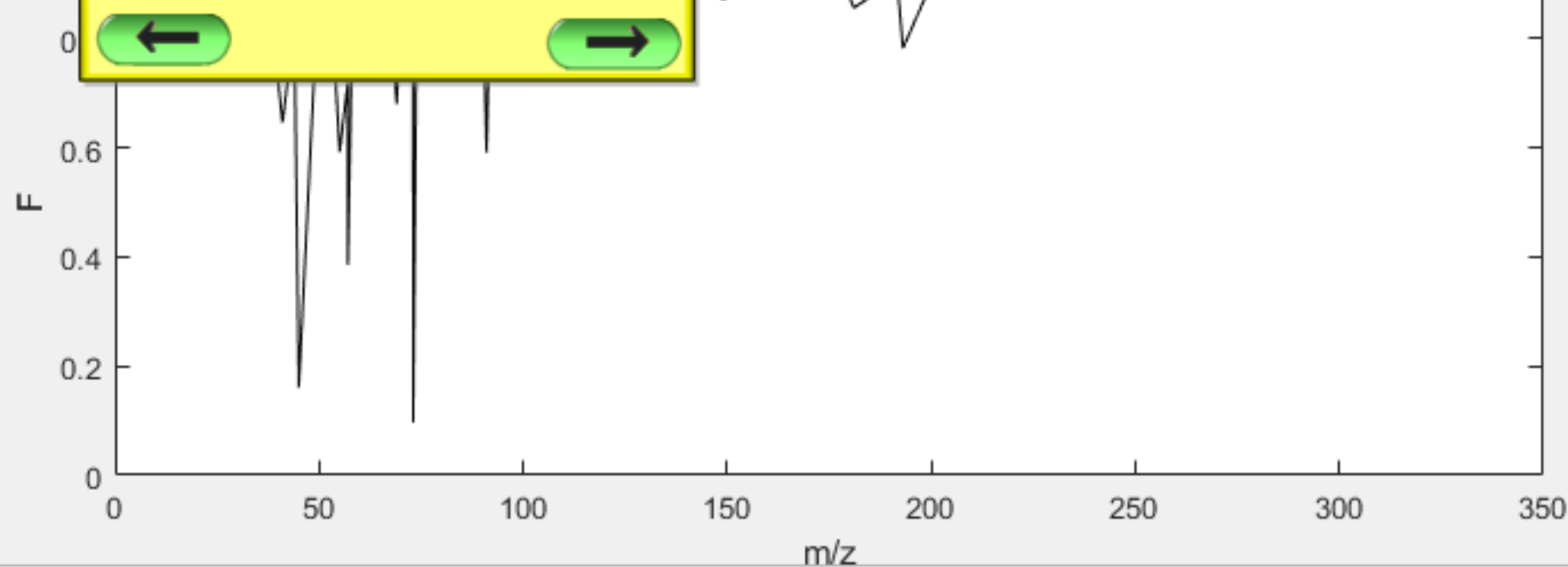
Original image data



Factor 15 scores



Press the 'Show Loadings Image' button to display the loadings for the selected factor number from the 'factors to use' drop down list.



Data Selection Panel

Name of Image Matrix

imagedata_S3_DE...

Name of Variable Matrix

exactmass_S3_DE...

Load Selected Data

Image: imagedata_S3_DE_

Variables: exactmass_S3_DE_

factors to use

15

Use MSF

Peak List

15.0261
26.0143
27.0237
28.0311
29.0021
29.0397
31.0195
38.0138
39.0232
41.0401
43.0186
44.0254
45.0376
50.0148
51.0238
52.0305
53.0397

Plot MSF Eig Vals

Plot Lack of Fit (F)

Show Q Residuals

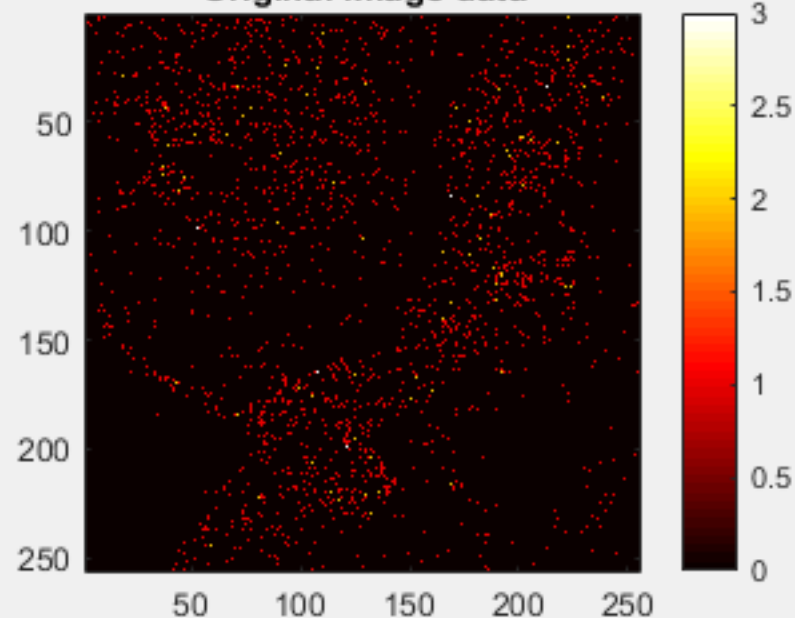
Show Sel Image

Show Score Image

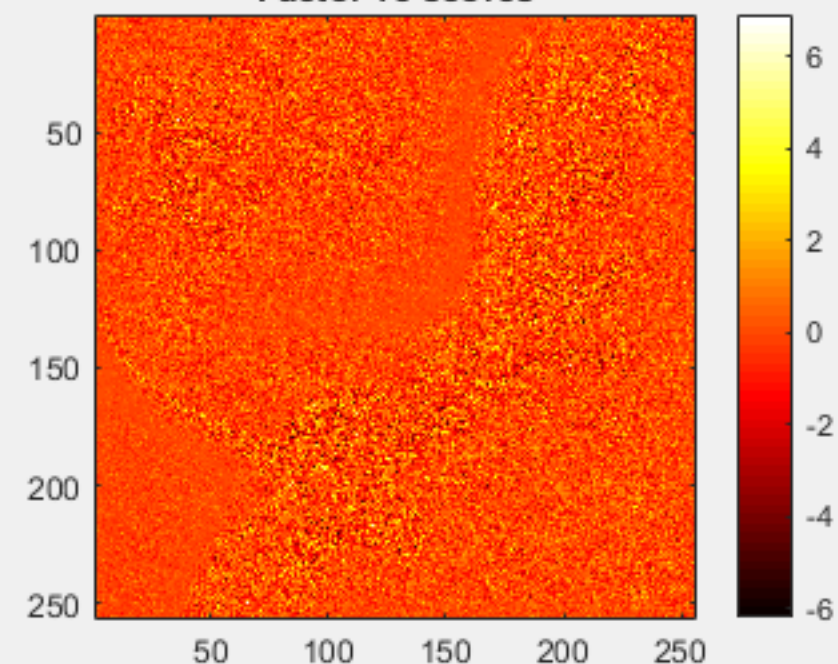
Show Loadings

Save Bottom Figure

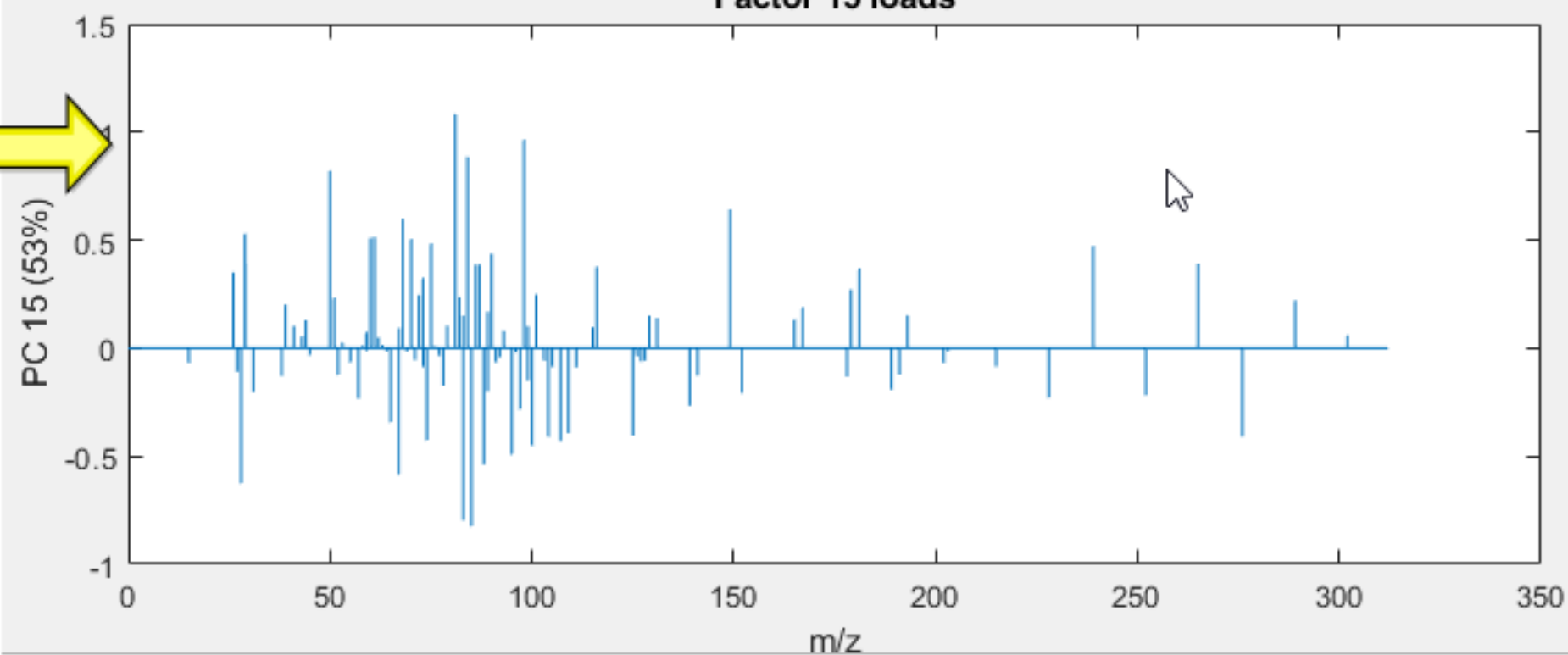
Original image data



Factor 15 scores



Factor 15 loads



The factor loadings will show up here plotted against the mass values of the variables (peaks).

Close

Data Selection Panel

Name of Image Matrix

imagedata_S3_DE...

Name of Variable Matrix

exactmass_S3_DE...

Load Selected Data

Image: imagedata_S3_DE_

Variables: exactmass_S3_DE_

factors to use

15

Use MSF

Peak List

15.0261
26.0143
27.0237
28.0311
29.0021
29.0397
31.0195
38.0138
39.0232
41.0401
43.0186
44.0254
45.0376
50.0148
51.0238
52.0305
53.0394
55.0552
57.0352
57.0705
58.0423
59.0141

Plot MSF Eig Vals

Plot Lack of Fit (F)

Show Q Residuals

Show Sel Image

Show Score Image

Show Loadings

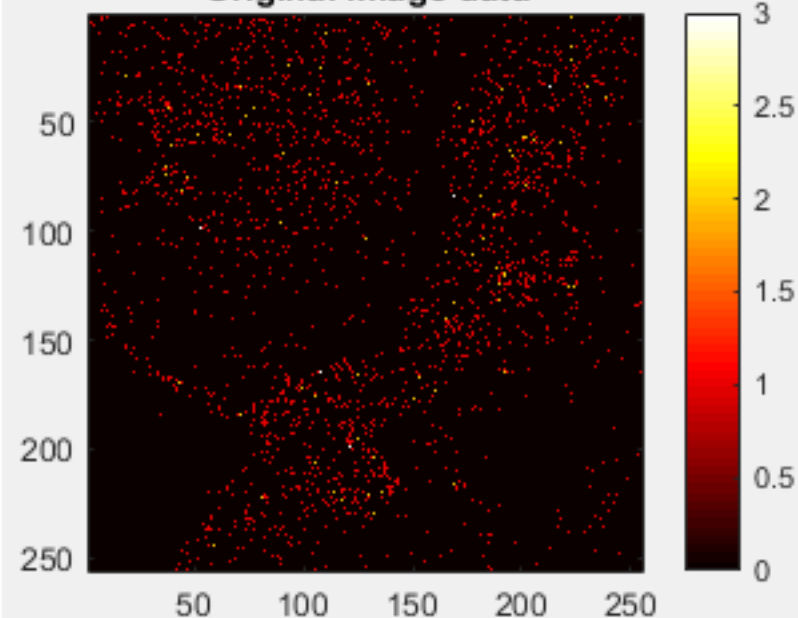
Save Bottom Figure

Save Left Image

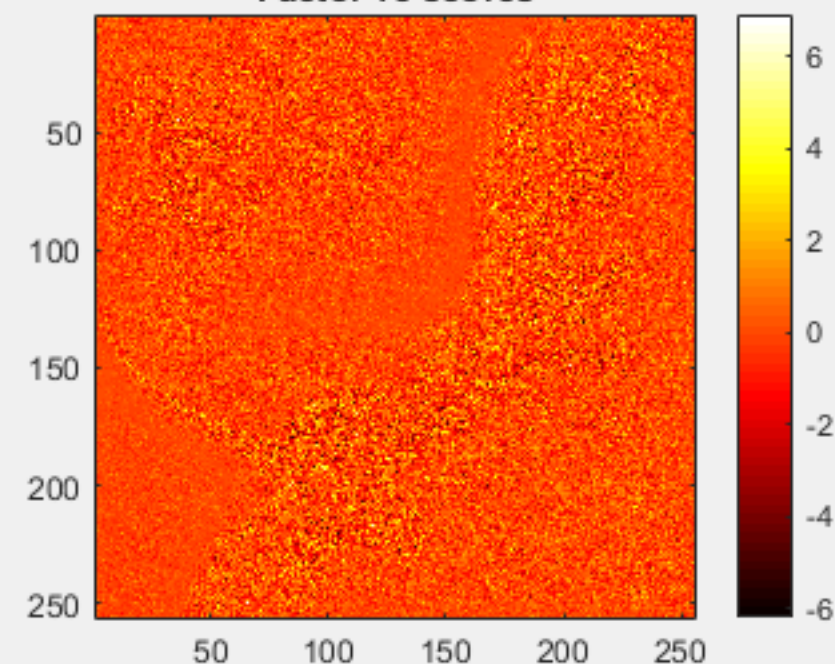
Save Right Image

Close

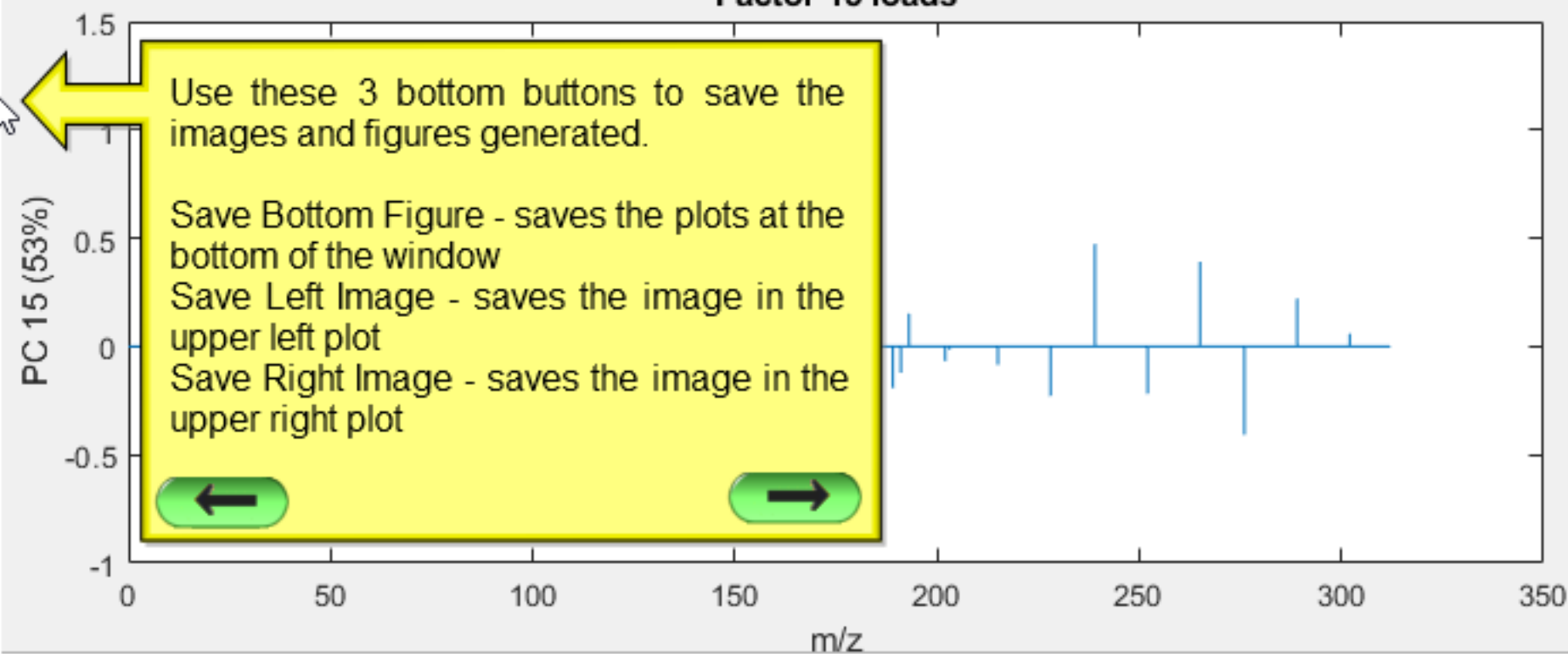
Original image data



Factor 15 scores



Factor 15 loads



Data Selection Panel

Name of Image Matrix

imagedata_S3_DE...

Name of Variable Matrix

exactmass_S3_DE...

Load Selected Data

Image: imagedata_S3_DE_

Variables: exactmass_S3_DE_

factors to use

15

Use MSF

Peak List

15.0261
26.0143
27.0237
28.0311
29.0021
29.0397
31.0195
38.0138
39.0232
41.0401
43.0186
44.0254
45.0376
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51.0238
52.0305
53.0394
55.0552
57.0352
57.0705
58.0423
59.0141

Plot MSF Eig Vals

Plot Lack of Fit (F)

Show Q Residuals

Show Sel Image

Show Score Image

Show Loadings

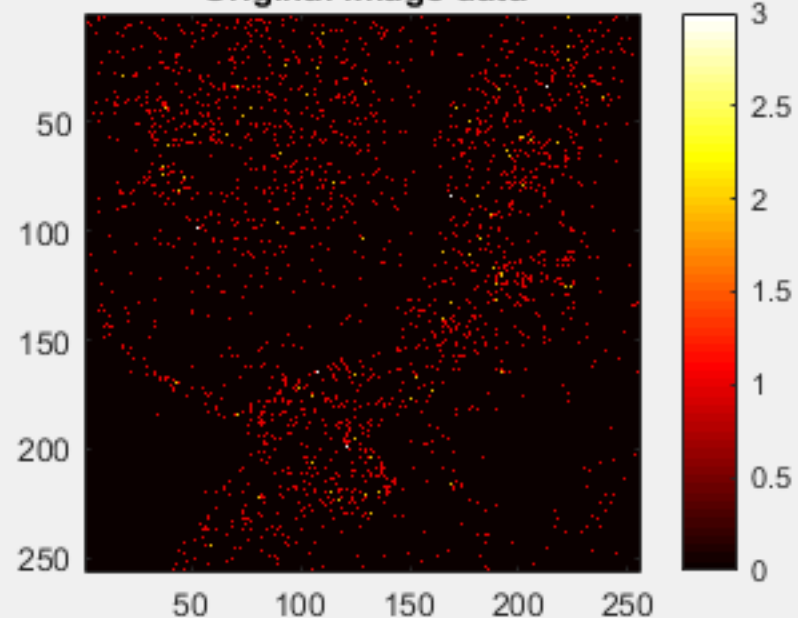
Save Bottom Figure

Save Left Image

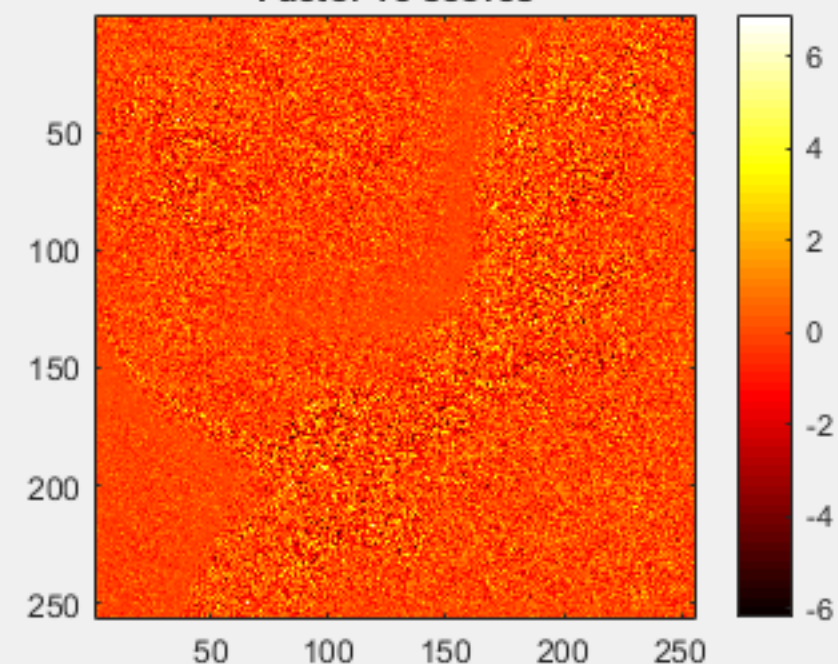
Save Right Image

Close

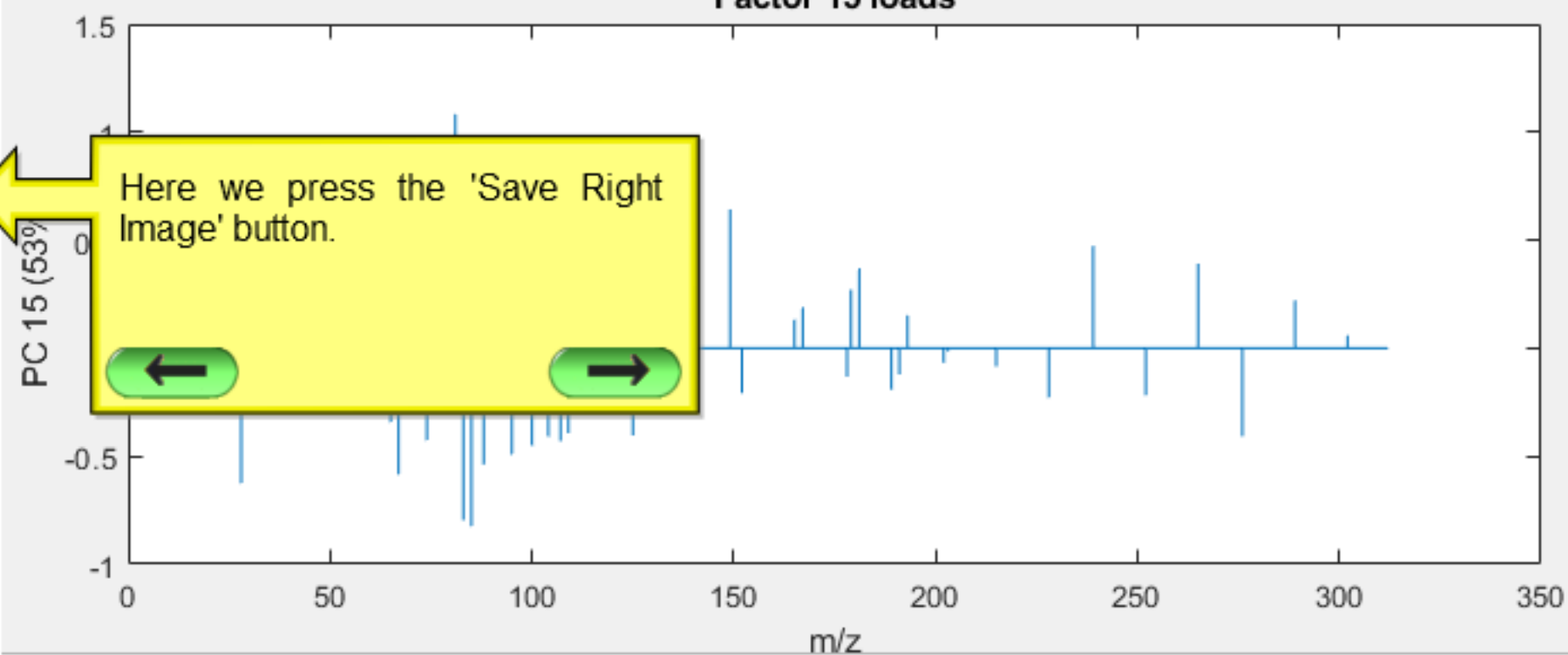
Original image data



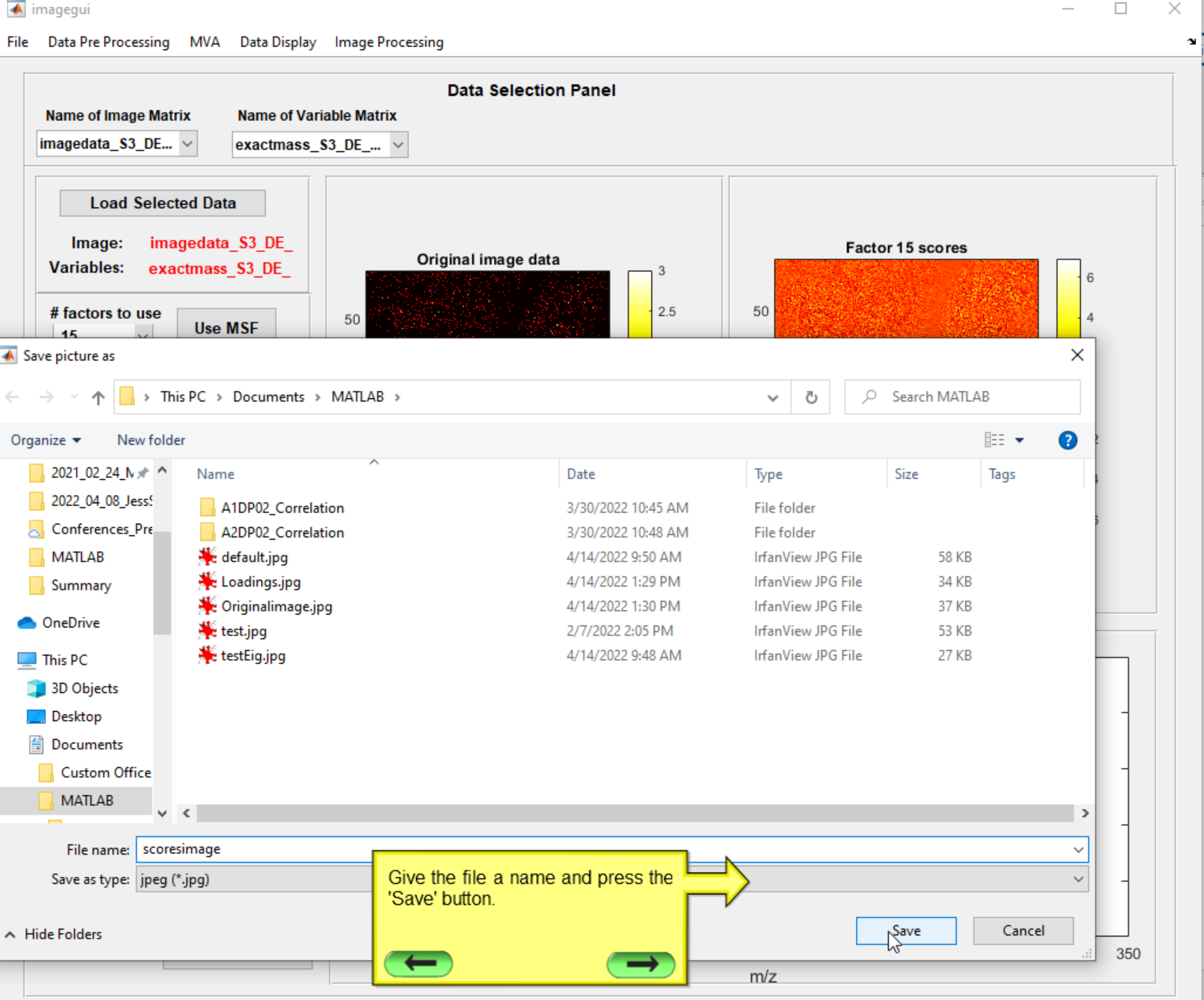
Factor 15 scores



Factor 15 loads



Here we press the 'Save Right Image' button.



Data Selection Panel

Name of Image Matrix

imagedata_S3_DE...

Name of Variable Matrix

exactmass_S3_DE_...

Load Selected Data

Image: imagedata_S3_DE_

Variables: exactmass_S3_DE_

factors to use

15

Use MSF

Choose...

1

2

3

4

5

6

7

8

9

10

11

12

13

14

15

16

17

18

19

Plot MSF Eig Vals

Plot Lack of Fit (F)

Show Q Residuals

Show Sel Image

Show

Sho

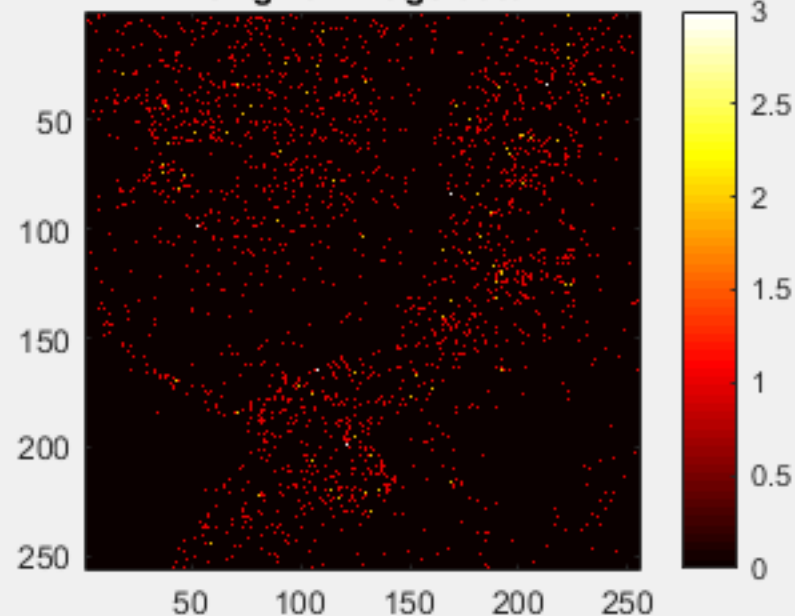
Save

Save

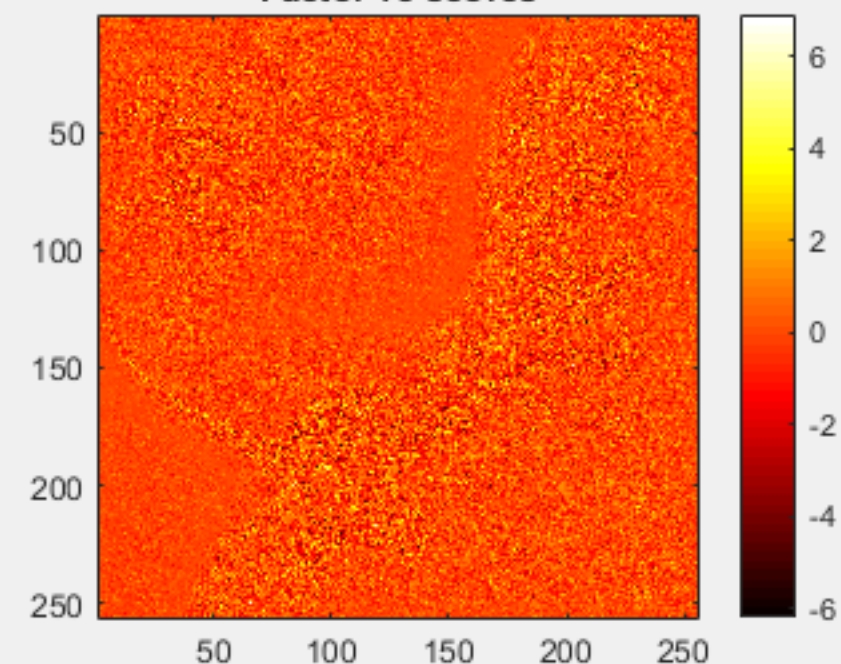
Save Right Image

Close

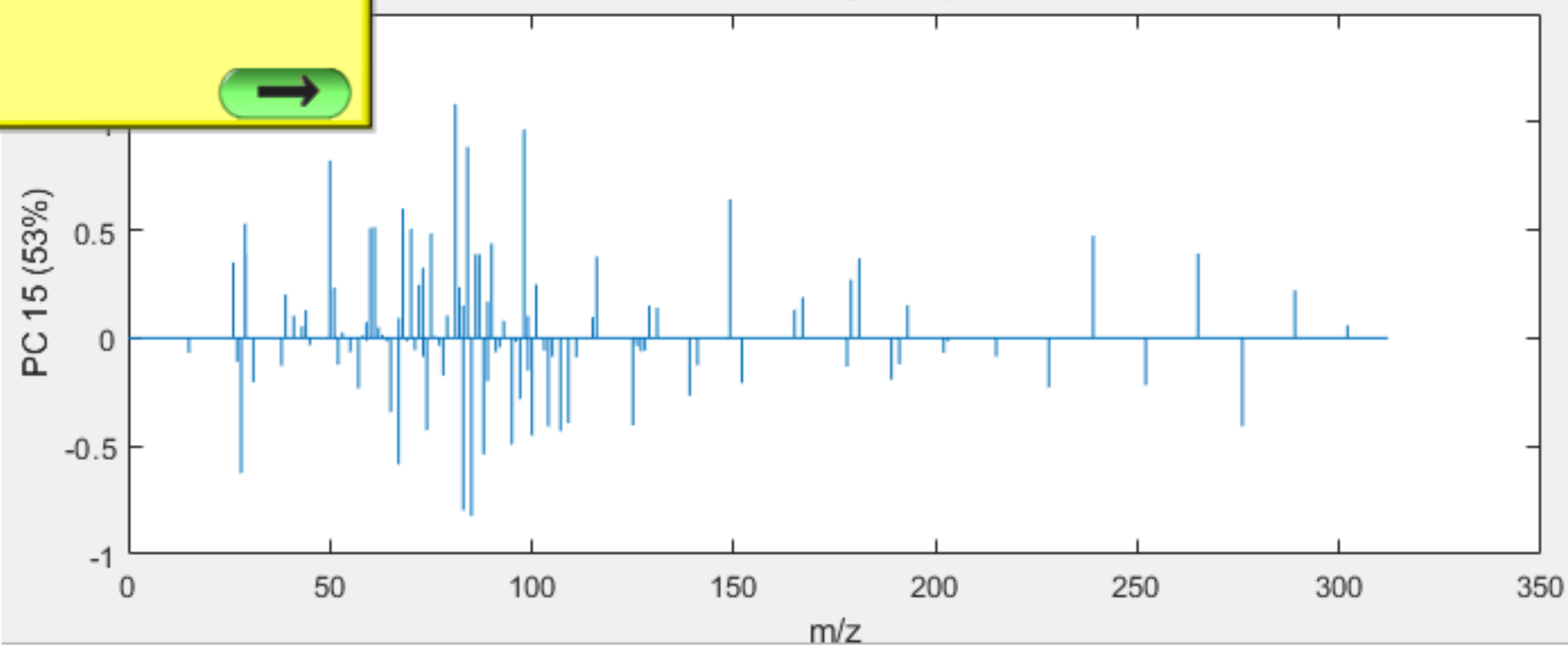
Original image data



Factor 15 scores



Factor 15 loads



To see the results for a different number of factors choose a new number from the drop down list.

Data Selection Panel

Name of Image Matrix

imagedata_S3_DE...

Name of Variable Matrix

exactmass_S3_DE...

Load Selected Data

Image: imagedata_S3_DE_

Variables: exactmass_S3_DE_

factors to use

10

Use MSF

Peak List

15.0261
26.0143
27.0237
28.0311
29.0021
29.0397
31.0195
38.0138
39.0232
41.0401
43.0186
44.0254
45.0376
50.0148
51.0238
52.0305
53.0394
55.0552
57.0352
57.0705
58.0423
59.0141

Plot MSF Eig Vals

Plot Lack of Fit (F)

Show Q Residuals

Show Sel Image

Show Score Image

Show Loadings

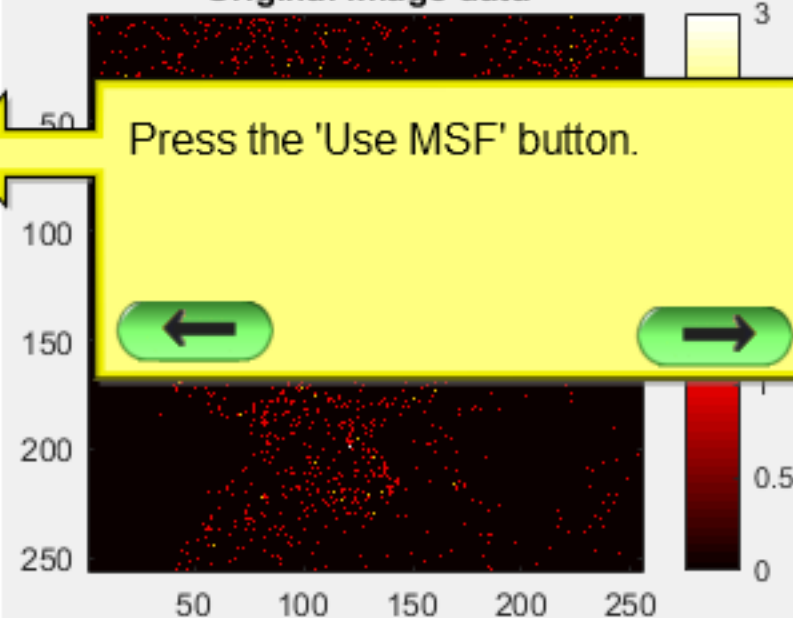
Save Bottom Figure

Save Left Image

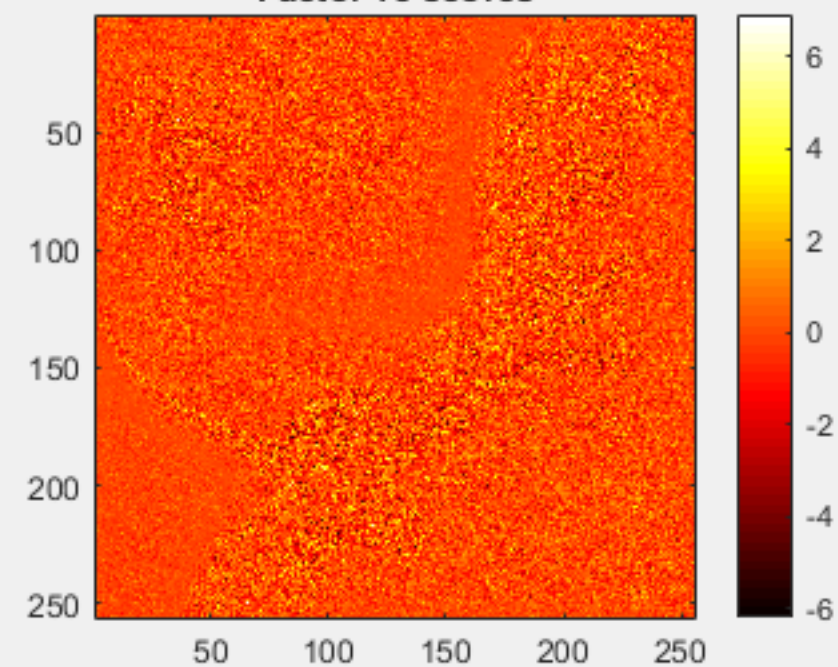
Save Right Image

Close

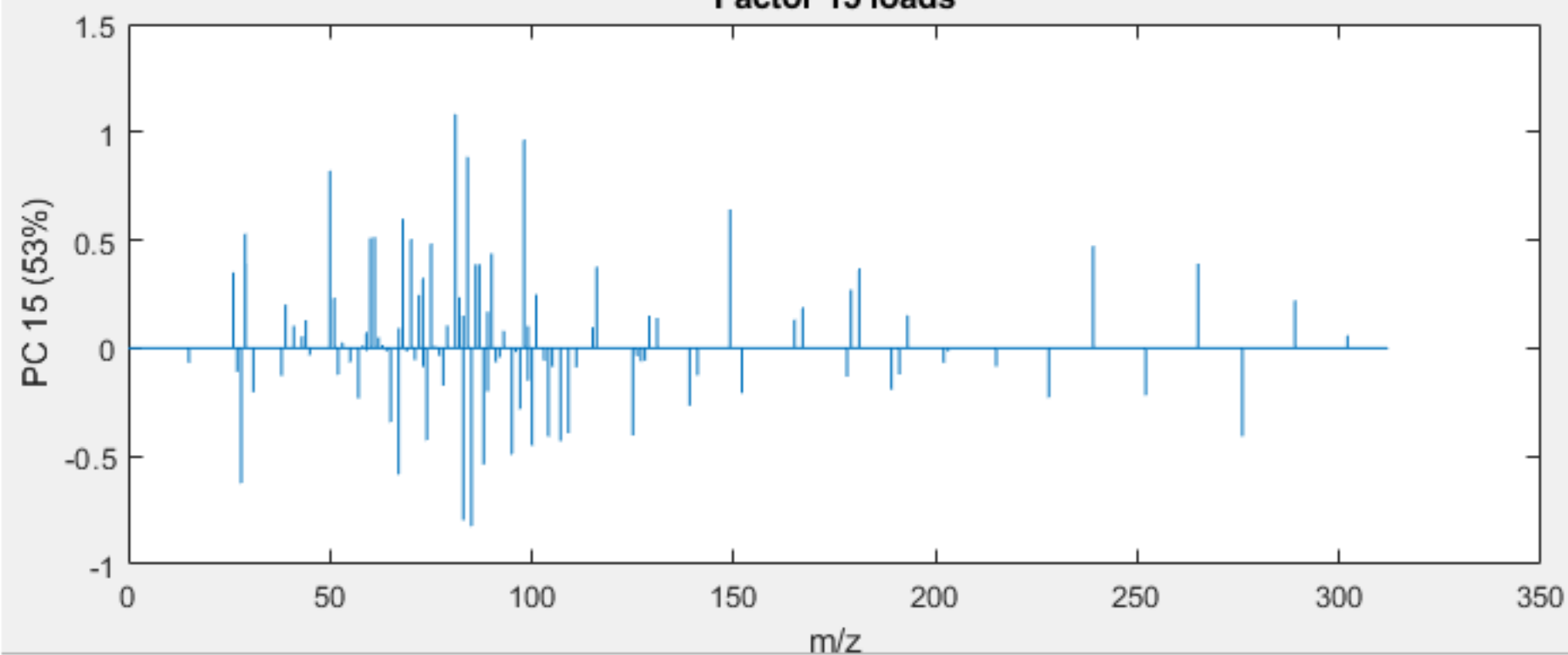
Original image data



Factor 15 scores



Factor 15 loads



Data Selection Panel

Name of Image Matrix

imagedata_S3_DE...

Name of Variable Matrix

exactmass_S3_DE...

Load Selected Data

Image: imagedata_S3_DE_

Variables: exactmass_S3_DE_

factors to use

15

Use MSF

Peak List

15.0261
26.0143
27.0237
28.0311
29.0021
29.0397
31.0195
38.0138
39.0232
41.0401
43.0186
44.0254
45.0376
50.0148
51.0238
52.0305
53.0394
55.0552
57.0352
57.0705
58.0423
59.0141

Plot MSF Eig Vals

Plot Lack of Fit (F)

Show Q Residuals

Show Sel Image

Show Score Image

Show Loadings

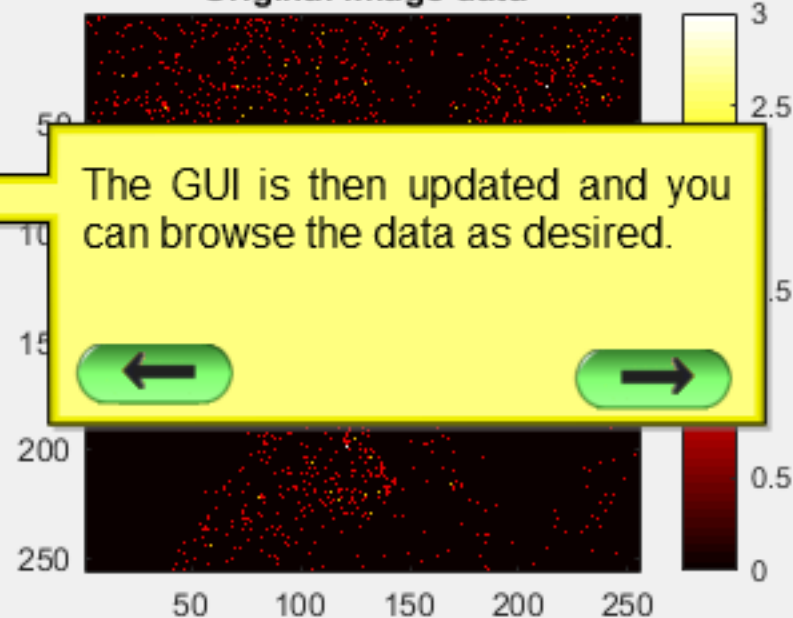
Save Bottom Figure

Save Left Image

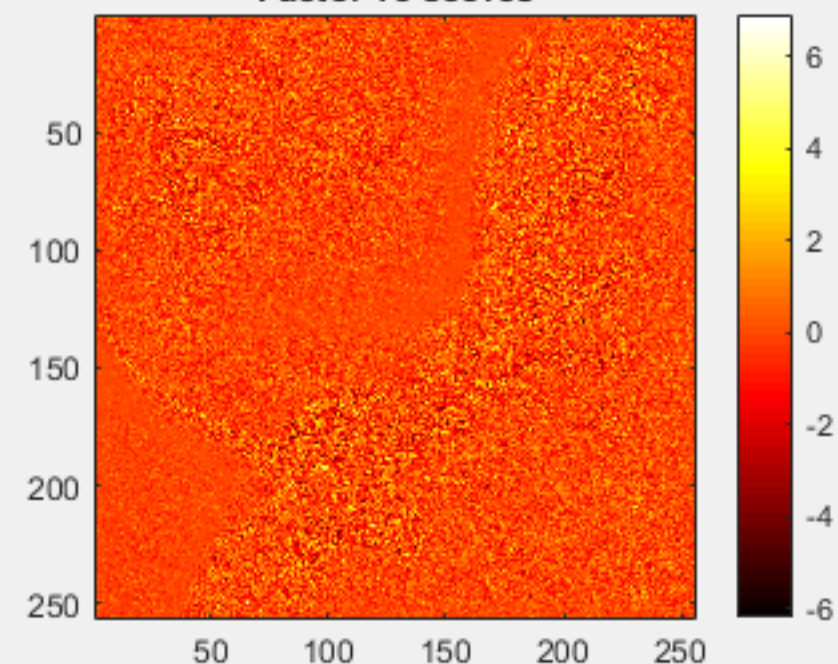
Save Right Image

Close

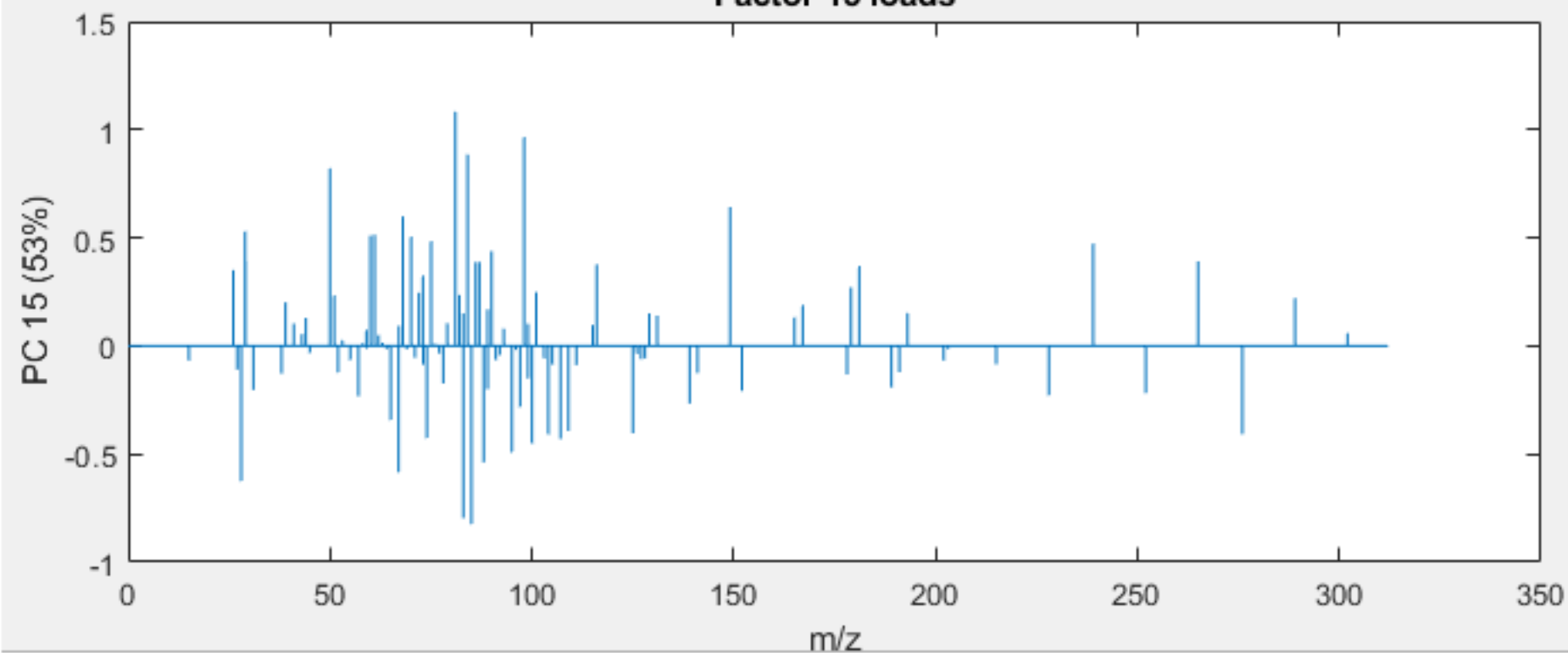
Original image data



Factor 15 scores



Factor 15 loads



Data Selection Panel

Name of Image Matrix

imagedata_S3_DE... ▾

Name of Variable Matrix

exactmass_S3_DE_... ▾

Load Selected Data

Image: imagedata_S3_DE_

Variables: exactmass_S3_DE_

factors to use

15 ▾

Use MSF

Peak List

15.0261
26.0143
27.0237
28.0311
29.0021
29.0397
31.0195
38.0138
39.0232
41.0401
43.0186
44.0254
45.0376
50.0148
51.0238
52.0305
53.0394
55.0552
57.0352
57.0705
58.0423
59.0141

Plot MSF Eig Vals

Plot Lack of Fit (F)

Show Q Residuals

Show Sel Image

Show Score Image

Show Loadings

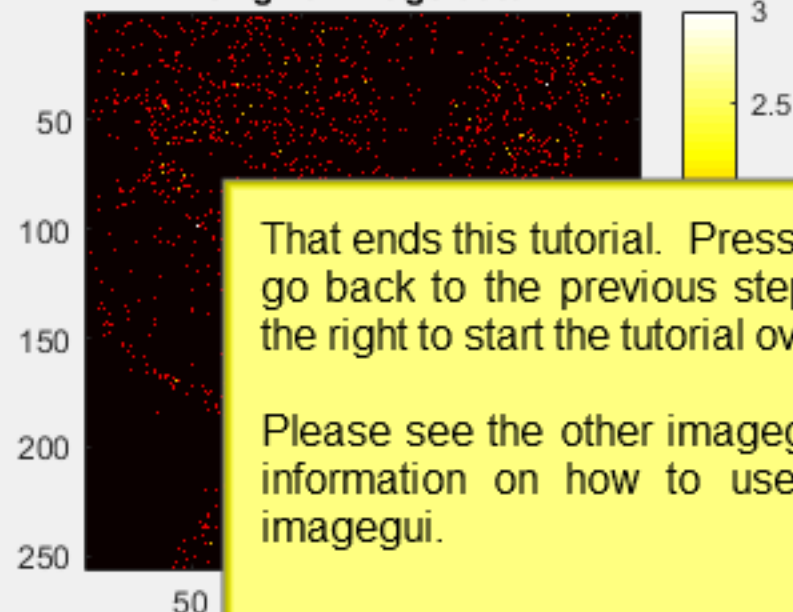
Save Bottom Figure

Save Left Image

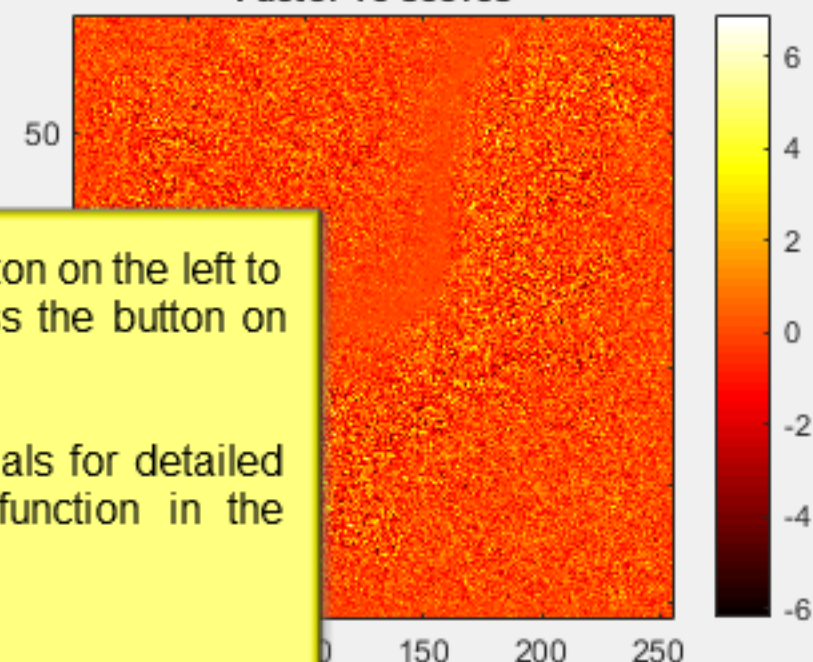
Save Right Image

Close

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