UNIMORE
UNIVERSITÀ DEGLI STUDI DI MODENA E REGGIO EMILIA
Dipartimento di Scienze della Vita

CHIMSLAB
Chemometrics Imaging and Spectroscopy Lab

HYPERSPECTROGRAMS

GUI V1.0:

FAST USER MANUAL

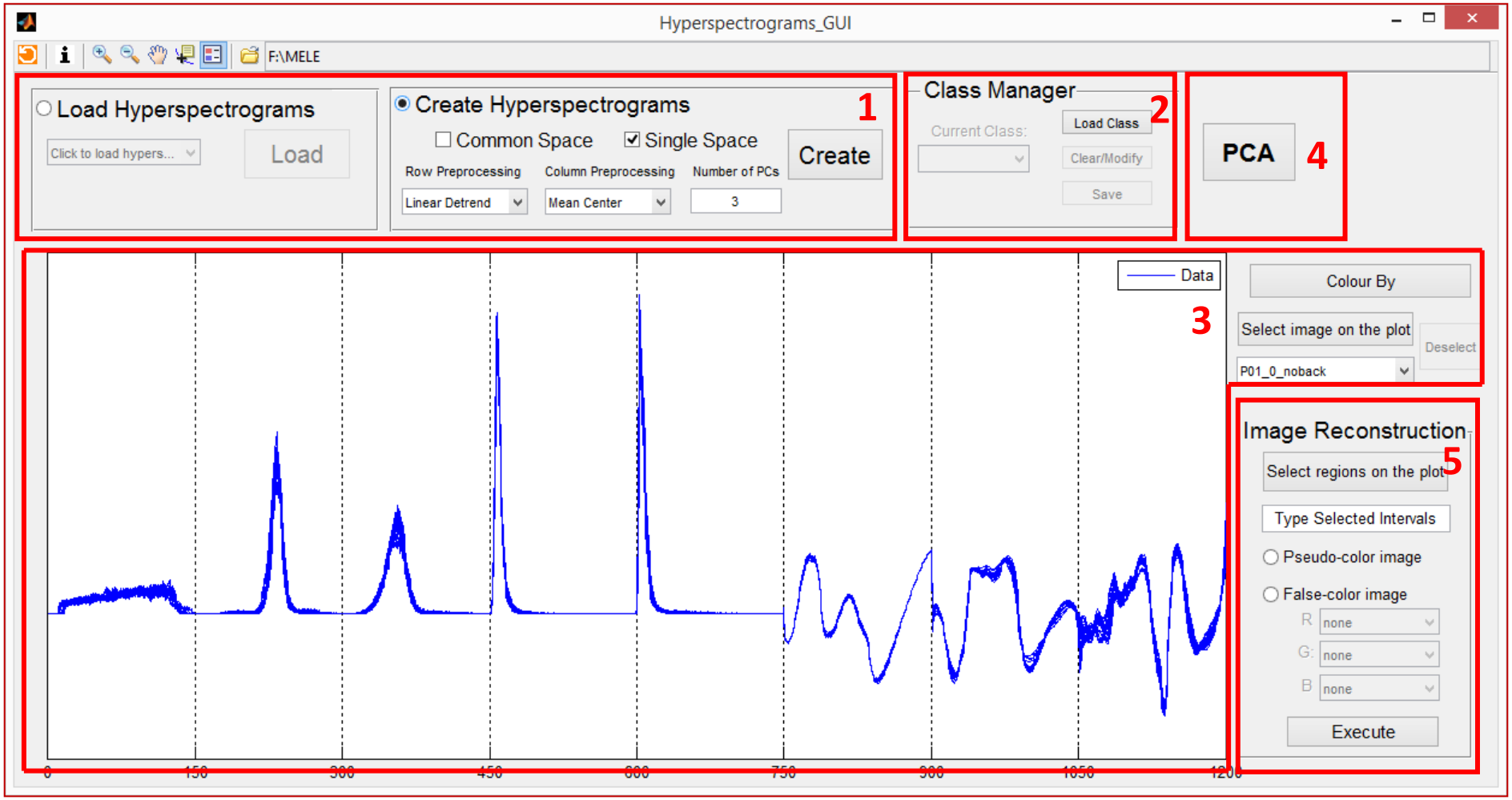
Getting started

Hyperspectrograms GUI can be easily installed in few steps:

1. Unzip the folder “SoftwareHyperspectrogramsGUI”.
2. Download the zip file of the DataSet Object from this link: http://se.mathworks.com/matlabcentral/fileexchange/39336-dataset-object.
3. Unzip the folder “@dataset” and save it inside Hyperspectrograms GUI main folder “HyperspectrogramsGUI_1.0”.
4. Open MATLAB, add the folder “HyperspectrogramsGUI_1.0” and the corresponding subfolders to the MATLAB path (File -> Set path -> Add with subfolders).
5. To get started, type Hyperspectrograms_GUI in the MATLAB command window. The main window of Hyperspectrograms GUI will be displayed and ready to use!!

For any question, problem or technical assistance don’t hesitate to send us an e-mail at chimslab.unimore@gmail.com.

Hyperspectrograms GUI main window



1. Load or create hyperspectrograms dataset.
2. Add supplementary information.
3. Visualize signals.
4. Perform PCA.
5. Reconstruct images using features of interest.

Toolbar

1. Restart
2. Dataset Info
3. Zoom in
4. Zoom out
5. Pan
6. Data Cursor
7. Insert Legend
8. Select Folder

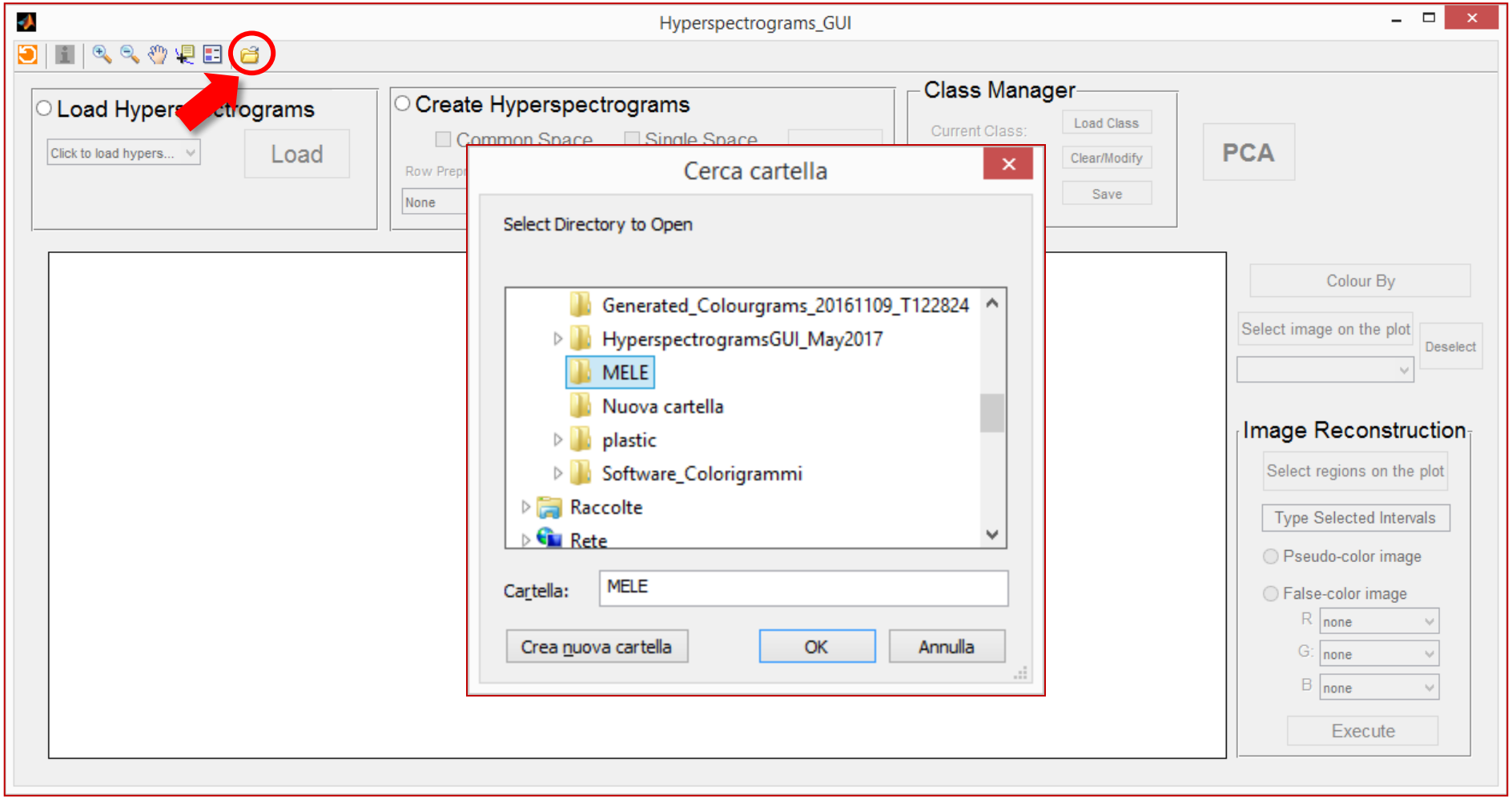
Restart

By clicking the “Restart” button, it is possible to start a new session.

Please, pay attention because this button **closes all figures.**

Select folder

By clicking on the folder icon in the toolbar, the user selects the folder containing the images to be converted into hyperspectrograms or a previously saved dataset. Once the current directory is selected, the corresponding path will be displayed in the toolbar.



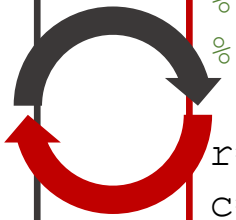
Create Hyperspectrograms

WARNING

HYPERSPECTROGRAMS GUI READS <u>ONLY</u> HYPERSPECTRAL IMAGES SAVED AS DATASET OBJECT.

```
%% From 3-D hypercube to DataSet
Object image:
% x -> 3-D hypercube
% wave -> vector of wavelengths
% x_dso -> DataSet Object image

[r,c,s]=size(x);
x_dso=dataset(reshape(x,r*c,s));
x_dso.type='image';
x_dso.imagesize=[r,c];
x_dso.axisscale{2,1}=wave;
```



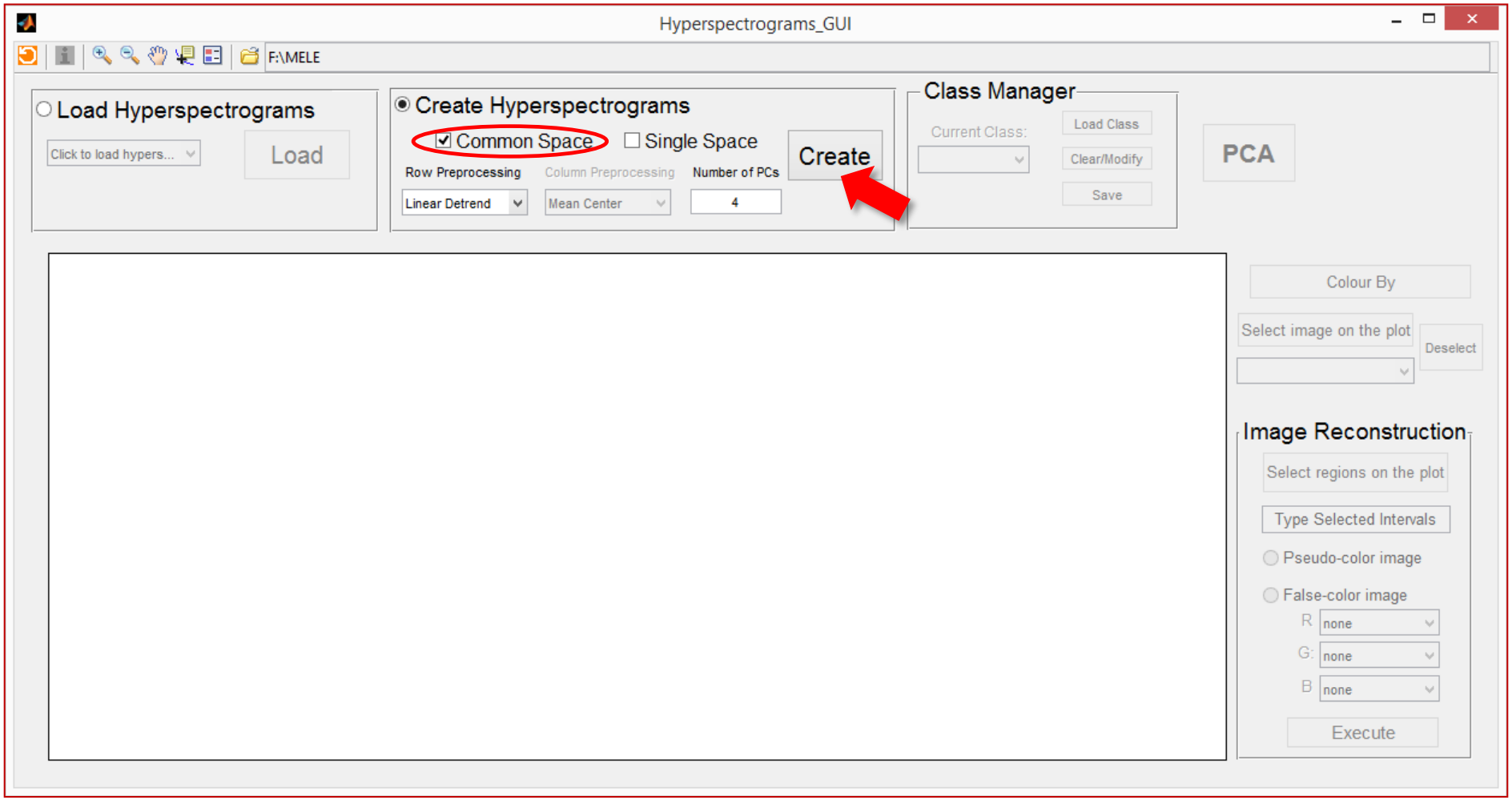
```
%% From DataSet Object image to
3-D hypercube:
% x_dso -> DataSet Object image
% x -> 3-D hypercube
% wave -> vector of wavelengths

r=x_dso.imagesize(1);
c=x_dso.imagesize(2);
s=size(x_dso,2);
x=reshape(x_dso.data,r,c,s);
wave=x_dso.axisscale{2,1};
```

For further details, contact us at: chimslab.unimore@gmail.com

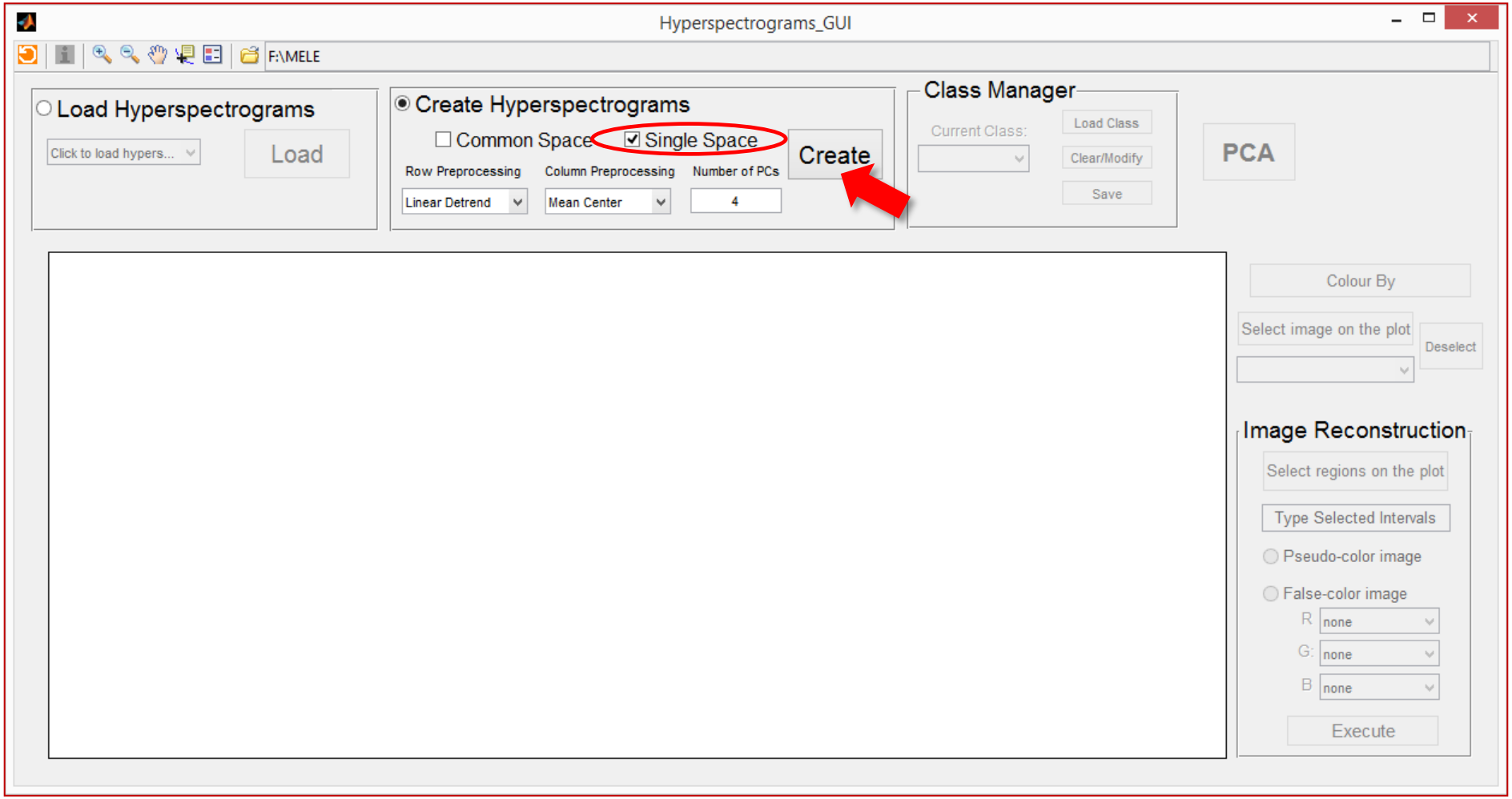
Create Hyperspectrograms – CSH

1. Define row preprocessing of spectra
2. Define the number of PCs
3. Click on Create button

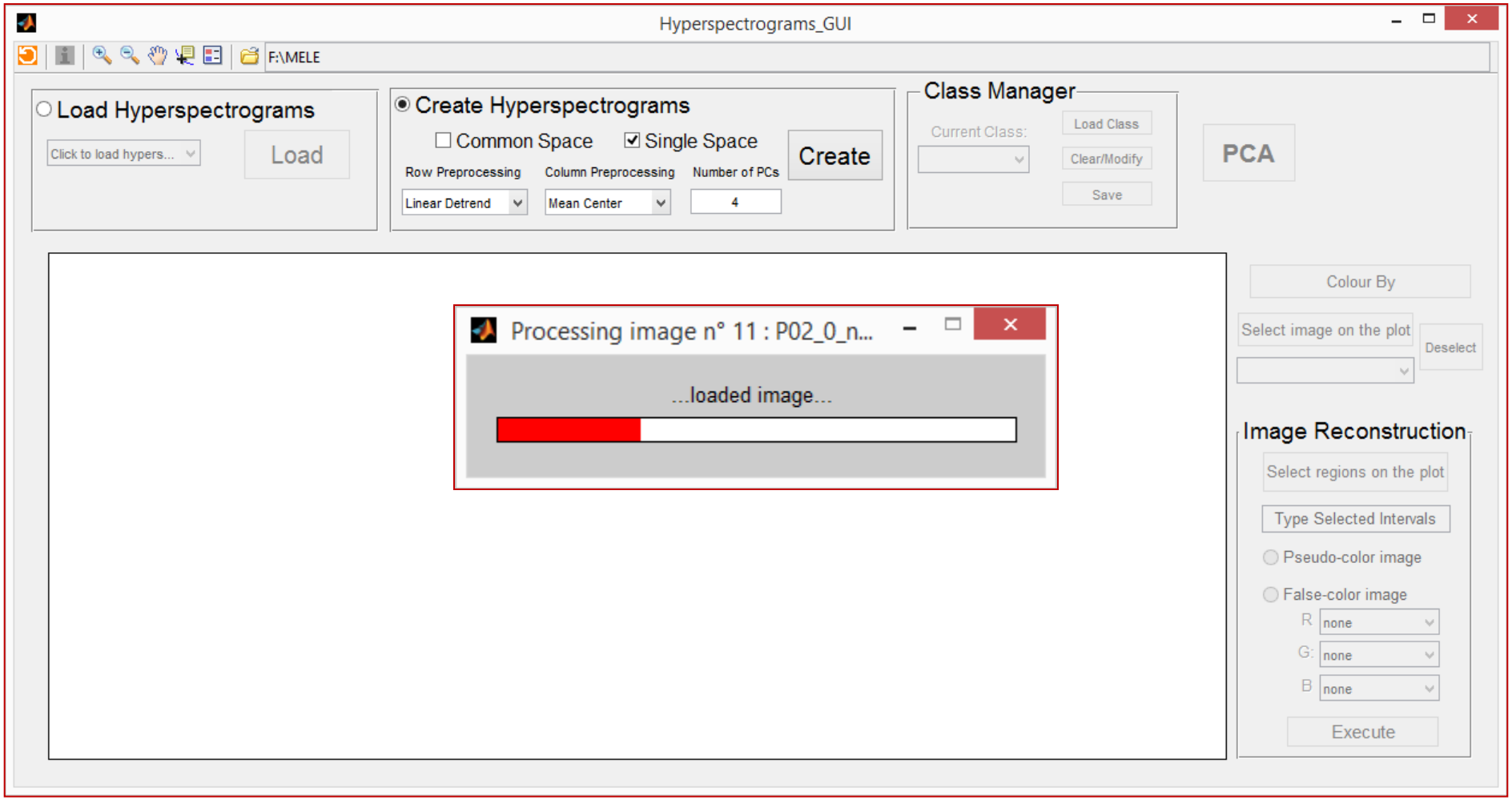


Create Hyperspectrograms – SSH

1. Define row <u>and column</u> preprocessing of spectra
2. Define the number of PCs
3. Click on Create button



Create Hyperspectrograms

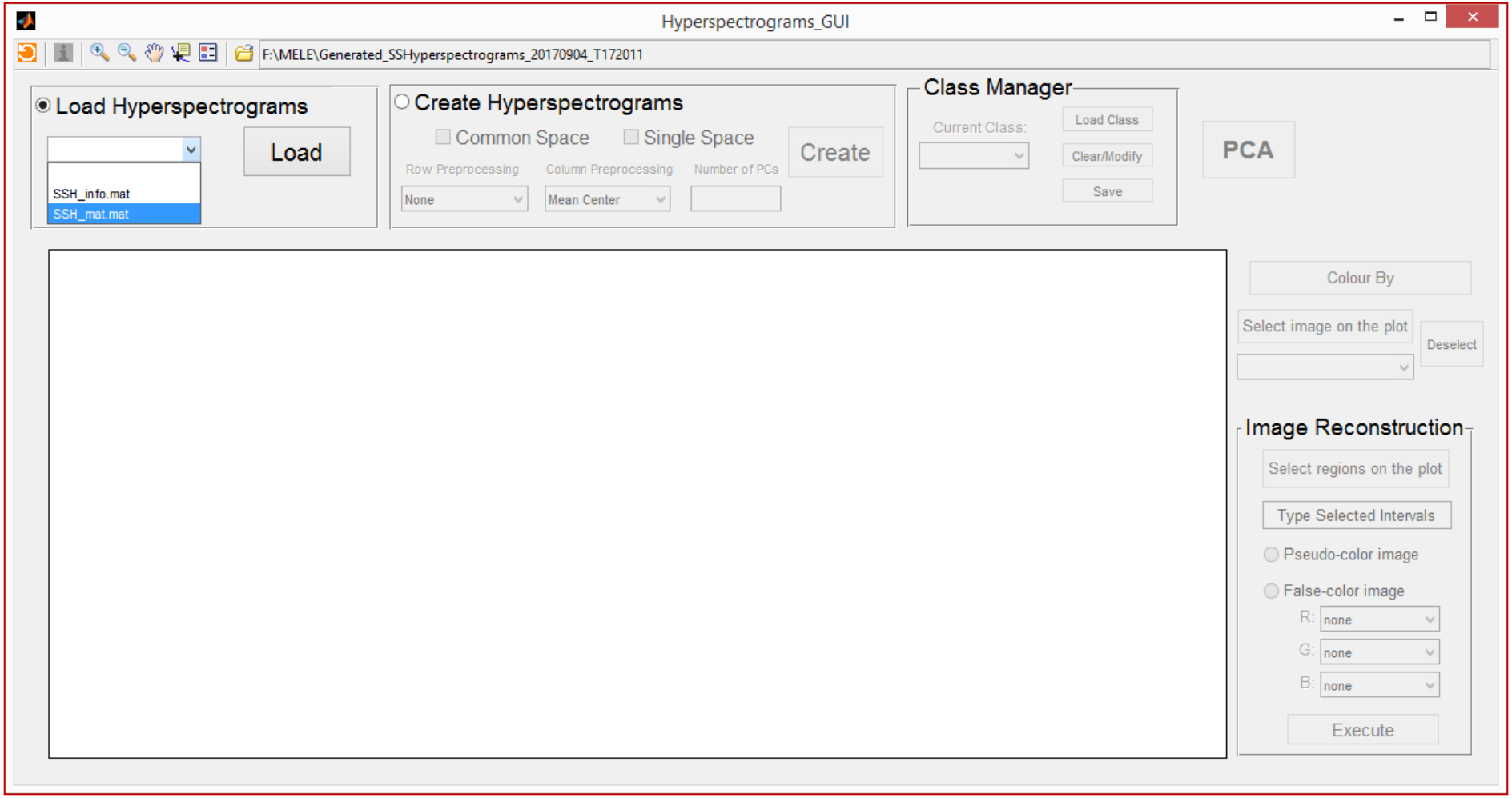


The hyperspectrograms are <u>automatically</u> saved as a DataSet Object.

In addition, also a MS-Excel file is saved, which contains the names of the original images and it can be used to note additional information about the dataset

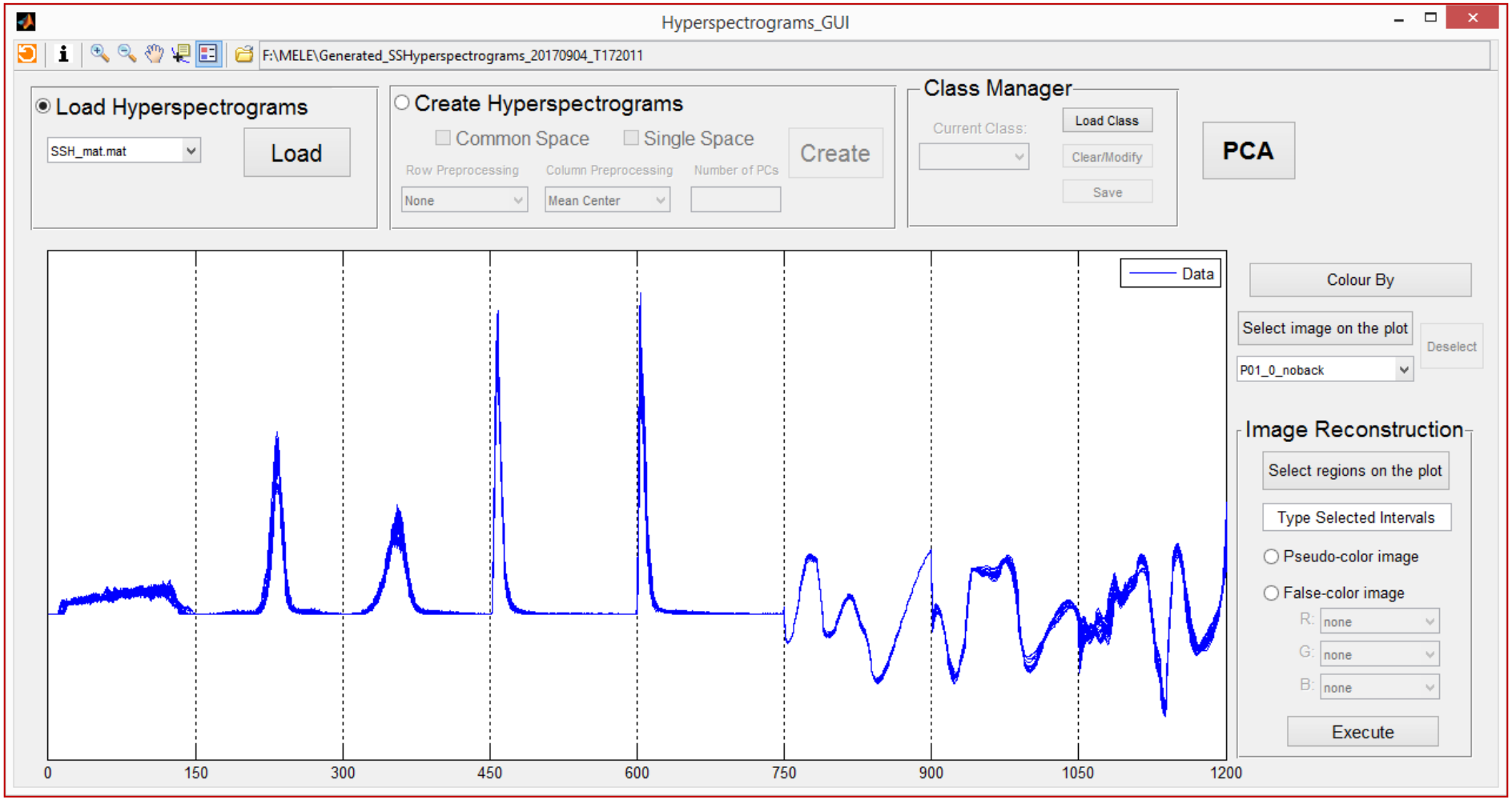
Load Hyperspectrograms

A previously saved DataSet Object of hyperspectrograms can be loaded by clicking on the radio button “Load Hyperspectrograms” and then selecting the corresponding file name from the pop-up menu.

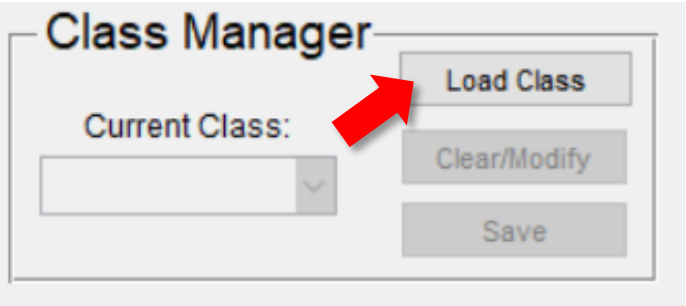


...ready to explore signals!!

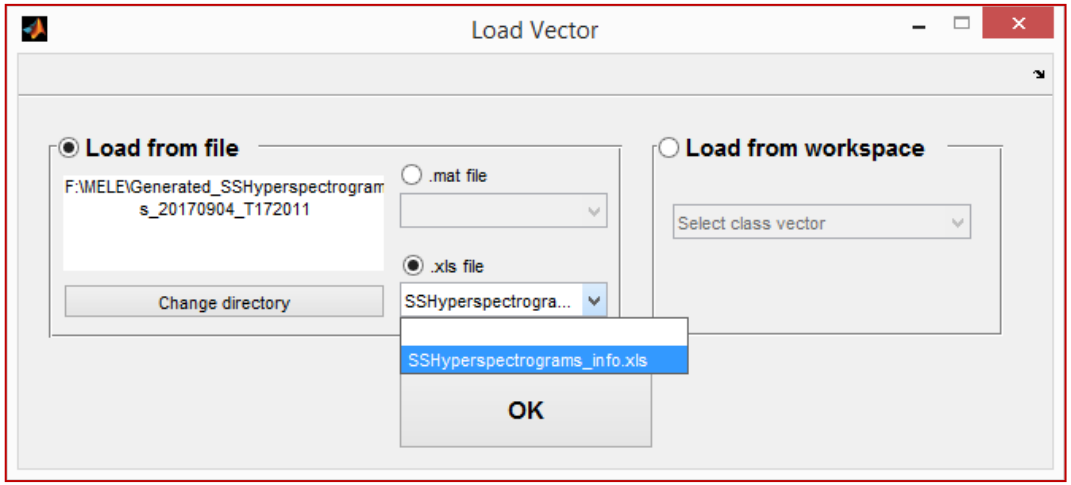
Once the hyperspectrograms are created or loaded, the signals are plotted on the main window and the tools for signal visualization and exploration are enabled.



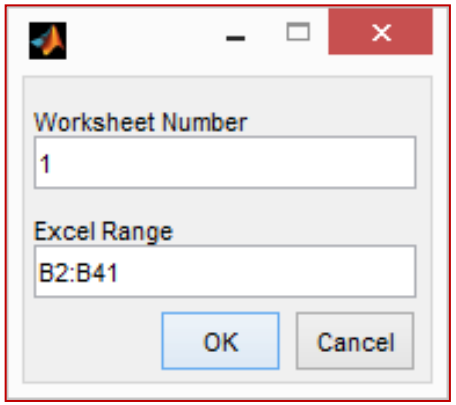
Class manager – Load Class



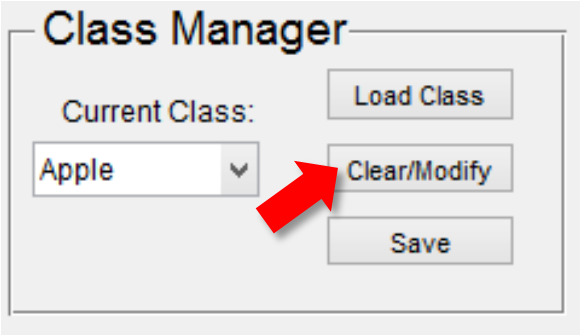
A new class vector can be loaded from a MATLAB **workspace variable**, from a **.mat file** or from a **.xls file**



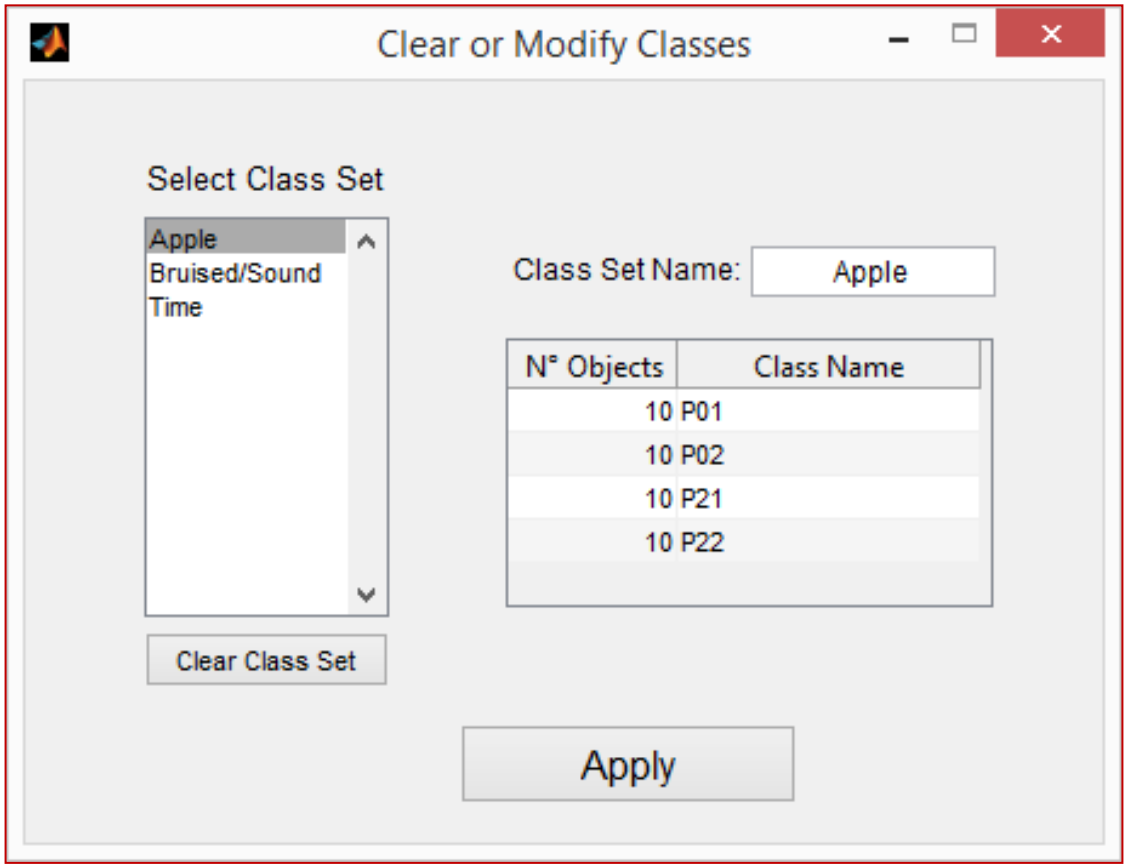
If the class vector is loaded from a .xls file, the user is required to specify the number of the Excel worksheet and the Excel range of the class vector



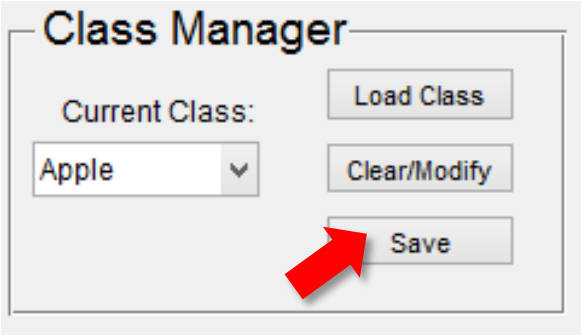
Class manager – Clear/Modify



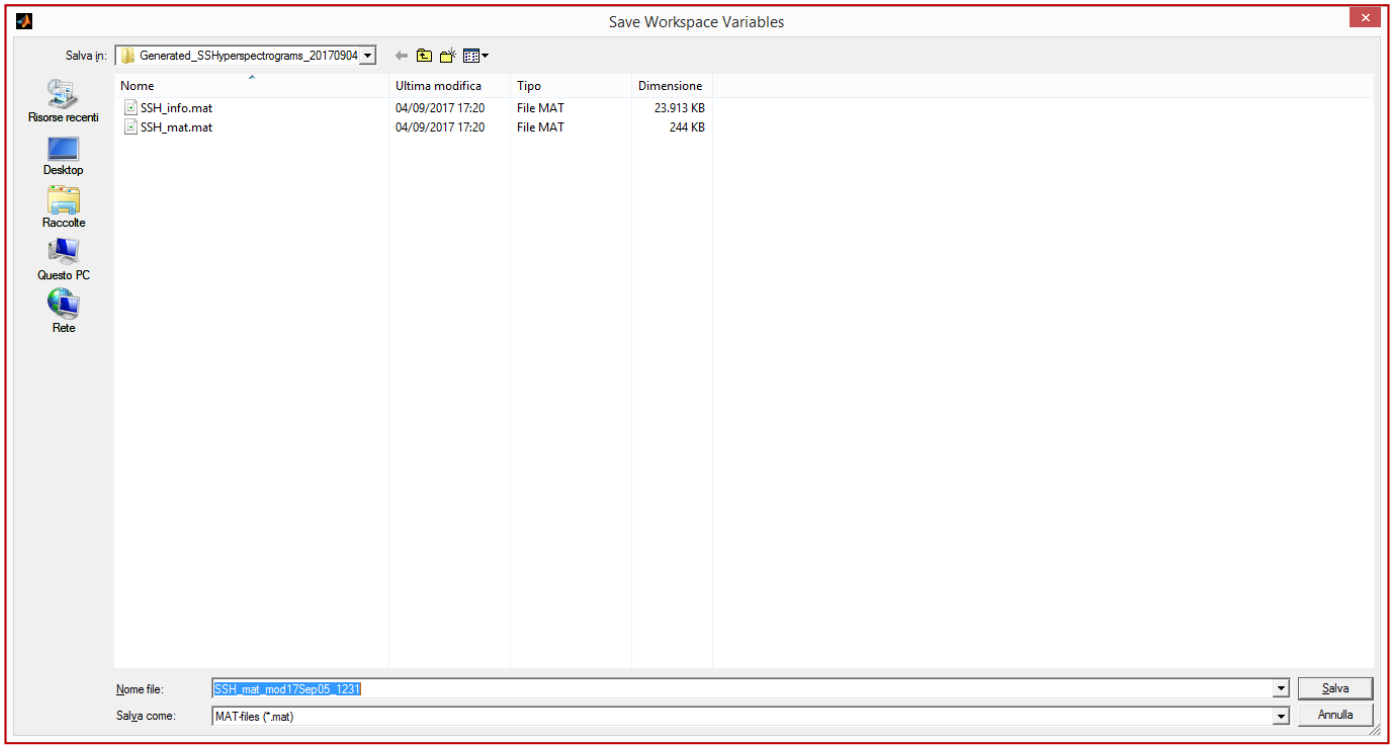
The push button “Clear/Modify” allows to clear or modify an existing class set.



Class manager - Save

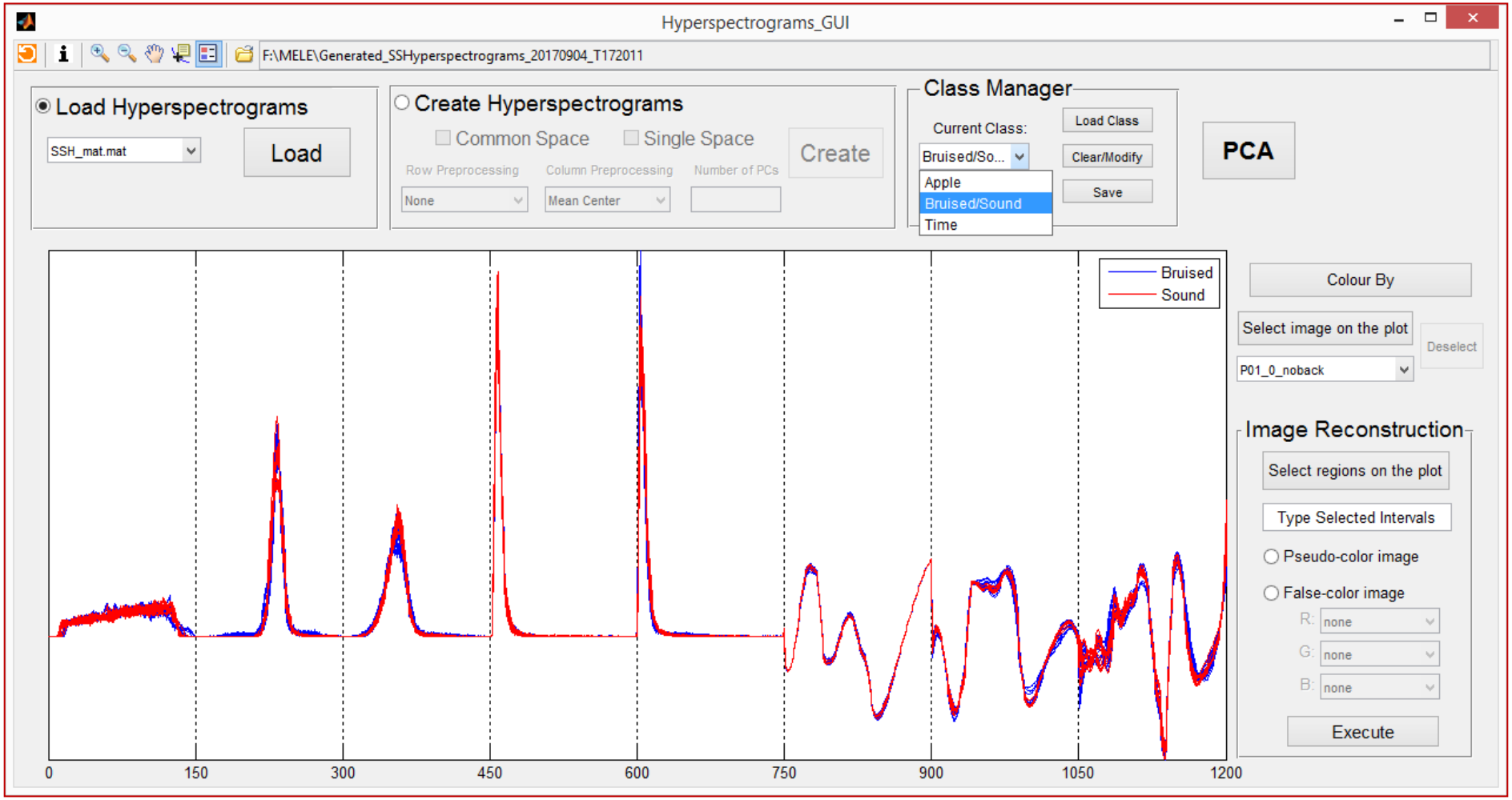


If the user has loaded new class sets, modified the names of existing classes or deleted a class set, the push button “Save” allows to save the updated DataSet Object to a .mat file.



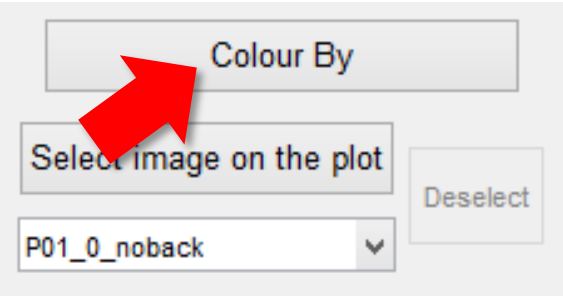
Class manager – Current Class

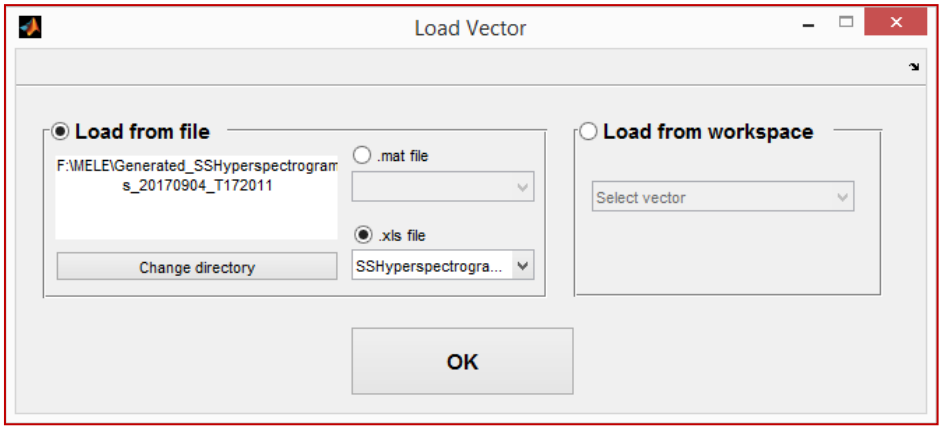
The “Current Class” pop-up menu of the “Class Manager” section allows to select the class identifiers set used to visualize the signals on the plot.

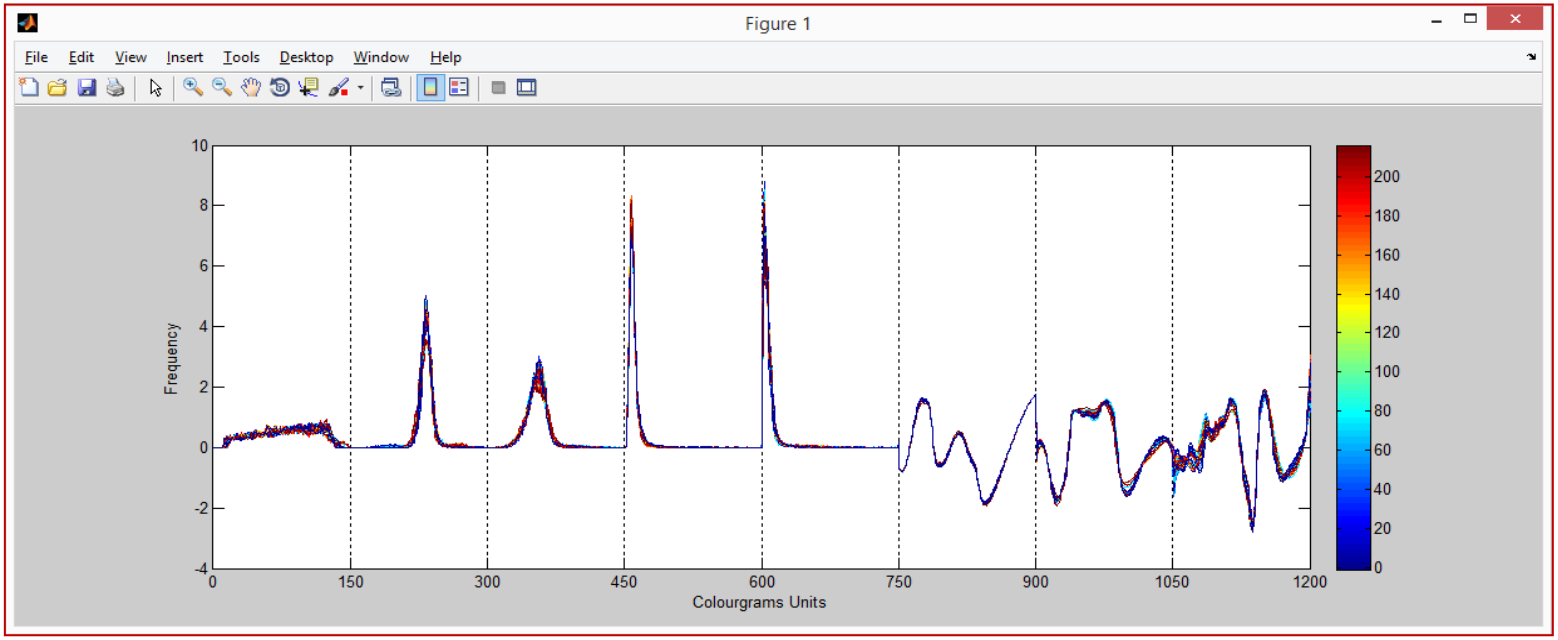


Visualize Signals

The “Colour By” push button allows to represent the hyperspectrograms according to a continuously varying quantitative property of the samples (e.g., concentration, time, etc..).







Visualize Signals

Identification and visualization of a specific signal.

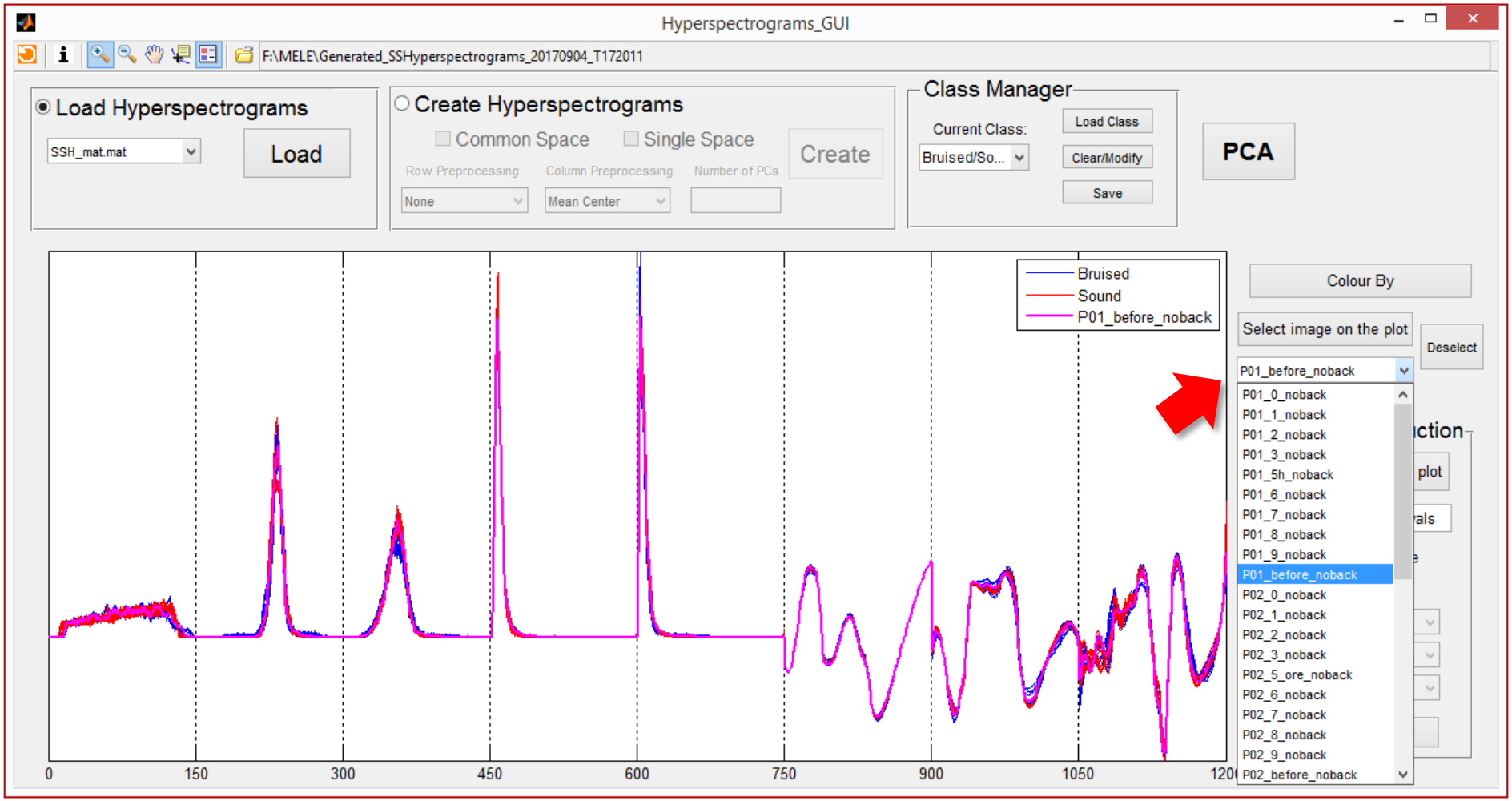


Image reconstruction

The user can either type the selected intervals in the edit box of the Hyperspectrograms GUI main window or click the “Select regions on the plot” push button to activate manual selection.

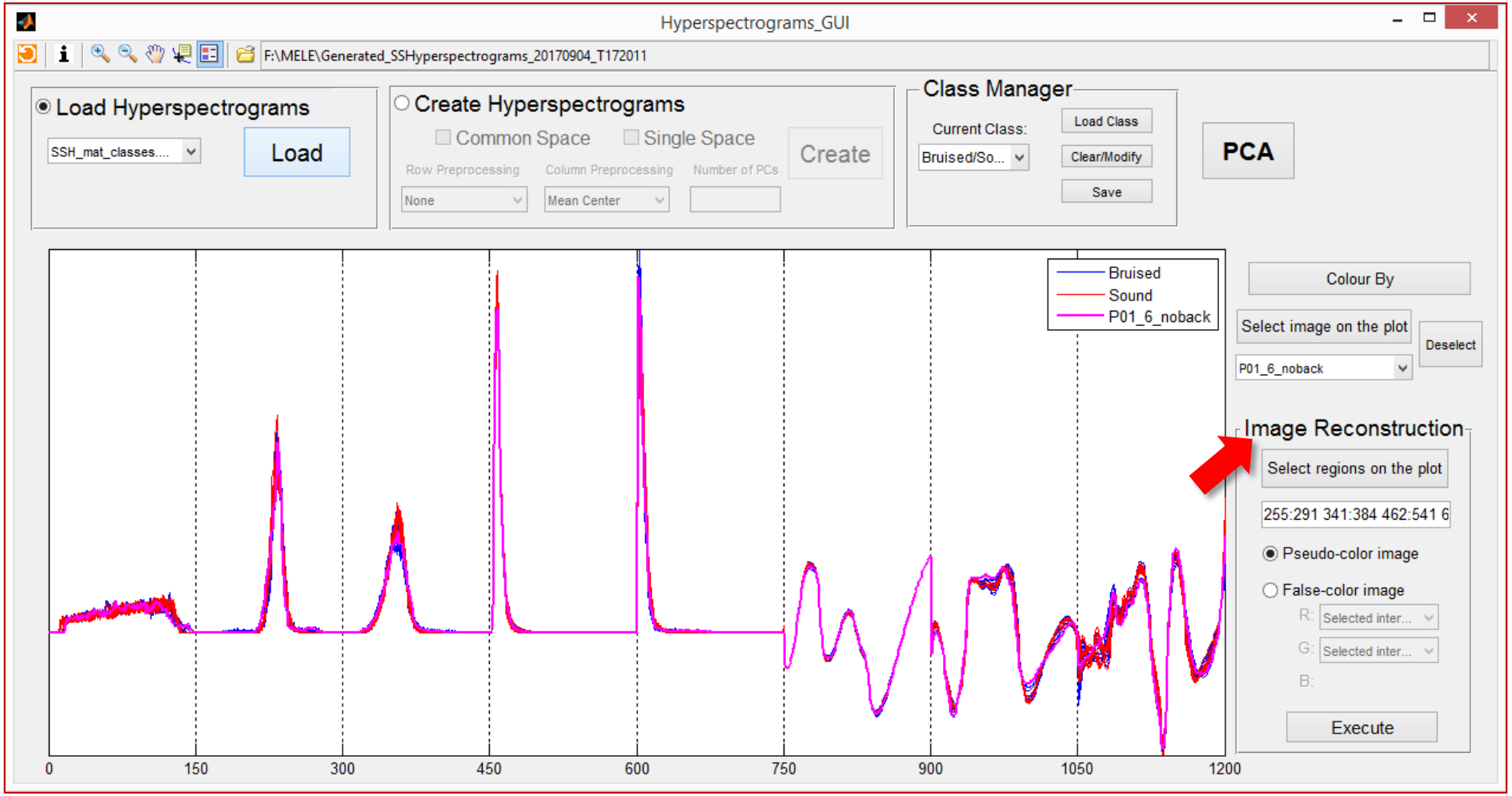


Image reconstruction: Pseudo-color image

For each frequency distribution curve where at least one interval has been chosen, a figure is obtained where only the pixels falling in the selected interval(s) are displayed, while the remainder pixels are represented in black colour.

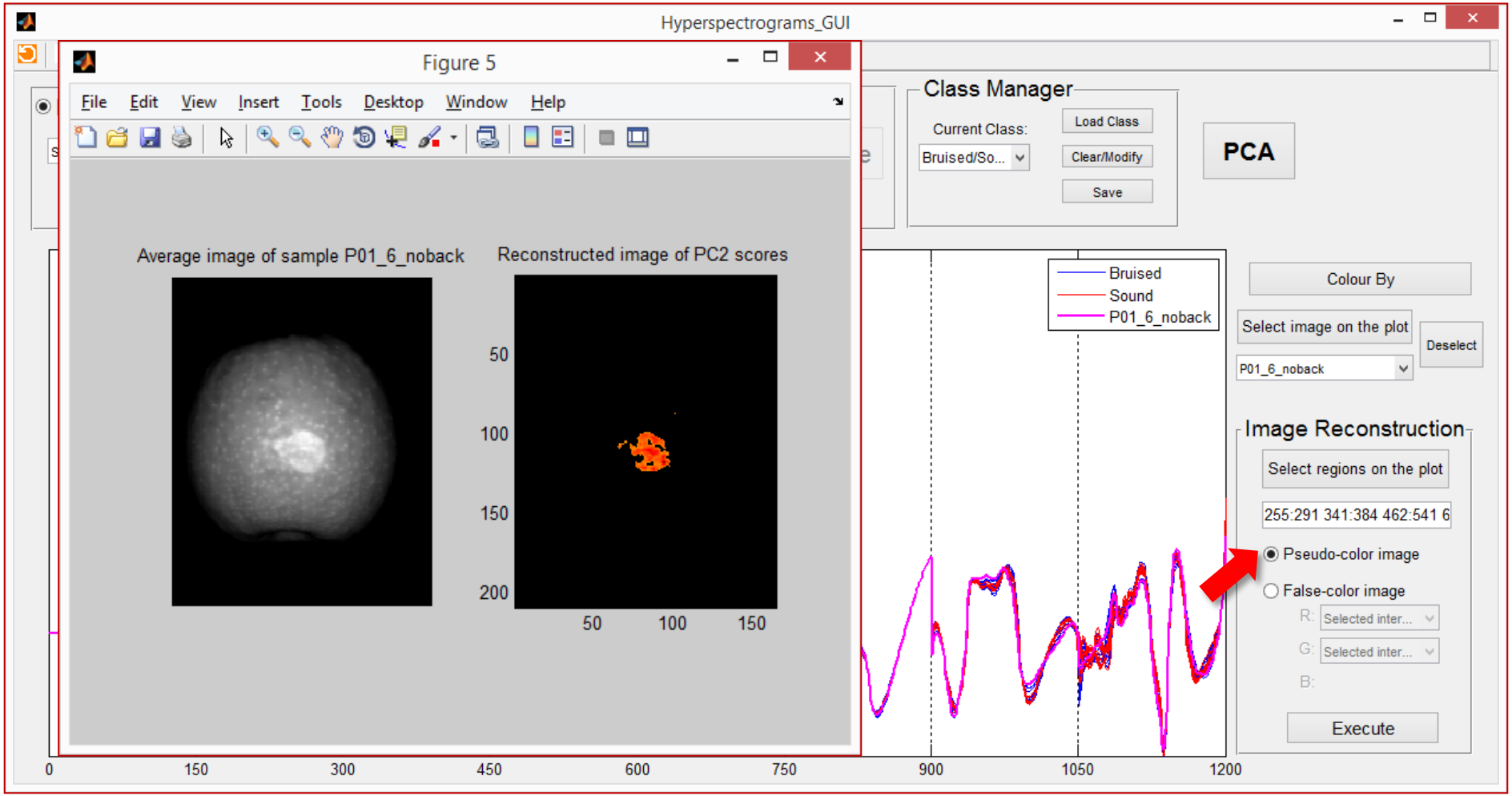
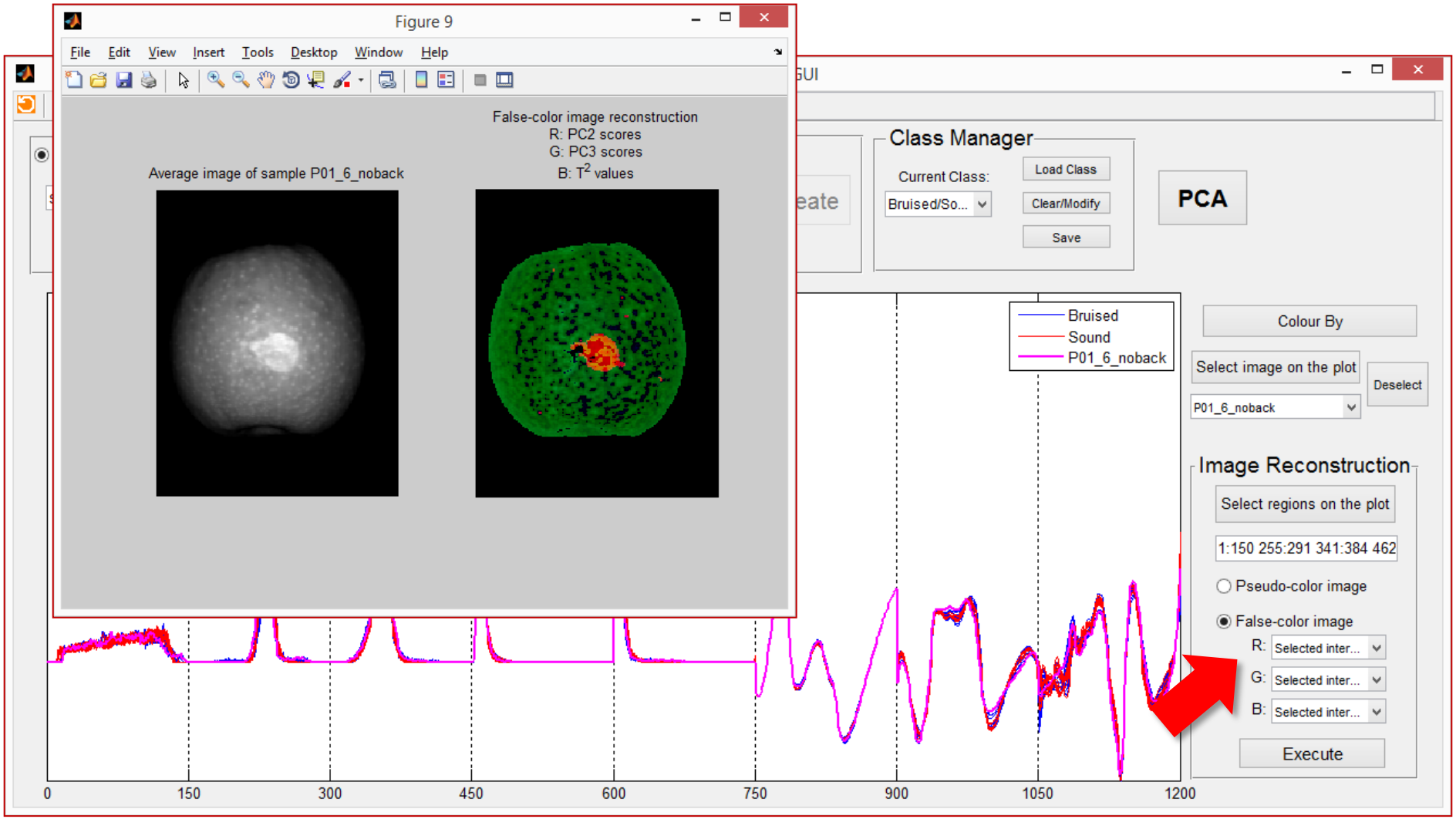


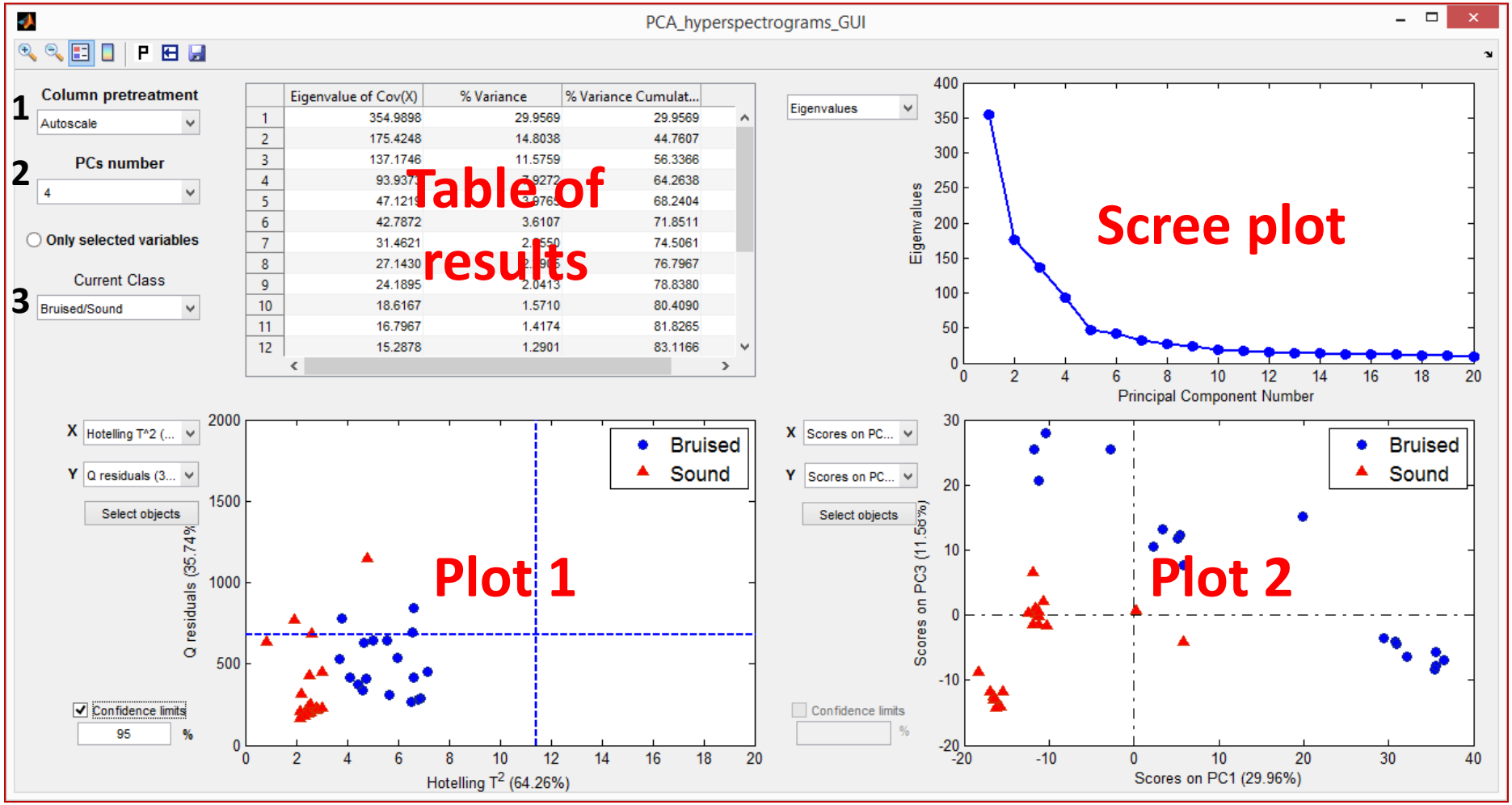
Image reconstruction: False-colour image

For each one of the R, G and B channels of the reconstructed false-colour image, the user can decide the selected interval(s) to be displayed.



PCA of the hyperspectrograms matrix

Click the **"PCA" button** of Hyperspectrograms GUI main window to display the PCA window.

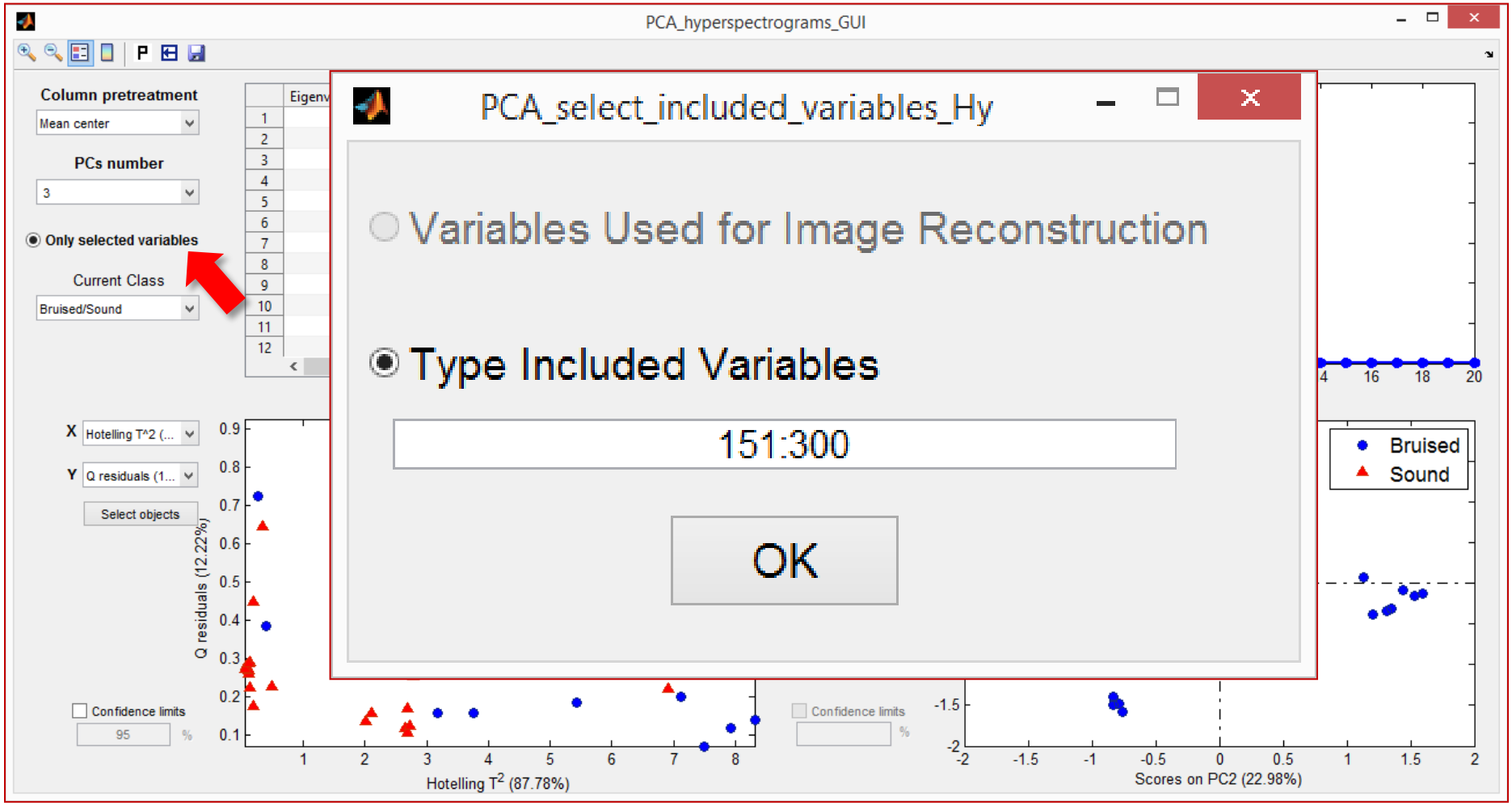


	Eigenvalue of Cov(X)	% Variance	% Variance Cumulat...
1	354.9898	29.9569	29.9569
2	175.4248	14.8038	44.7607
3	137.1746	11.5759	56.3366
4	93.937[illegible]	[illegible]	64.2638
5	47.121[illegible]	[illegible]	68.2404
6	42.7872	3.6107	71.8511
7	31.4621	[illegible]	74.5061
8	27.1430	[illegible]	76.7967
9	24.1895	2.0413	78.8380
10	18.6167	1.5710	80.4090
11	16.7967	1.4174	81.8265
12	15.2878	1.2901	83.1166

1. **Define signal preprocessing (mean center or autoscale)**
2. **Define the number of PCs**
3. **Select the class identifiers set used for object representation**

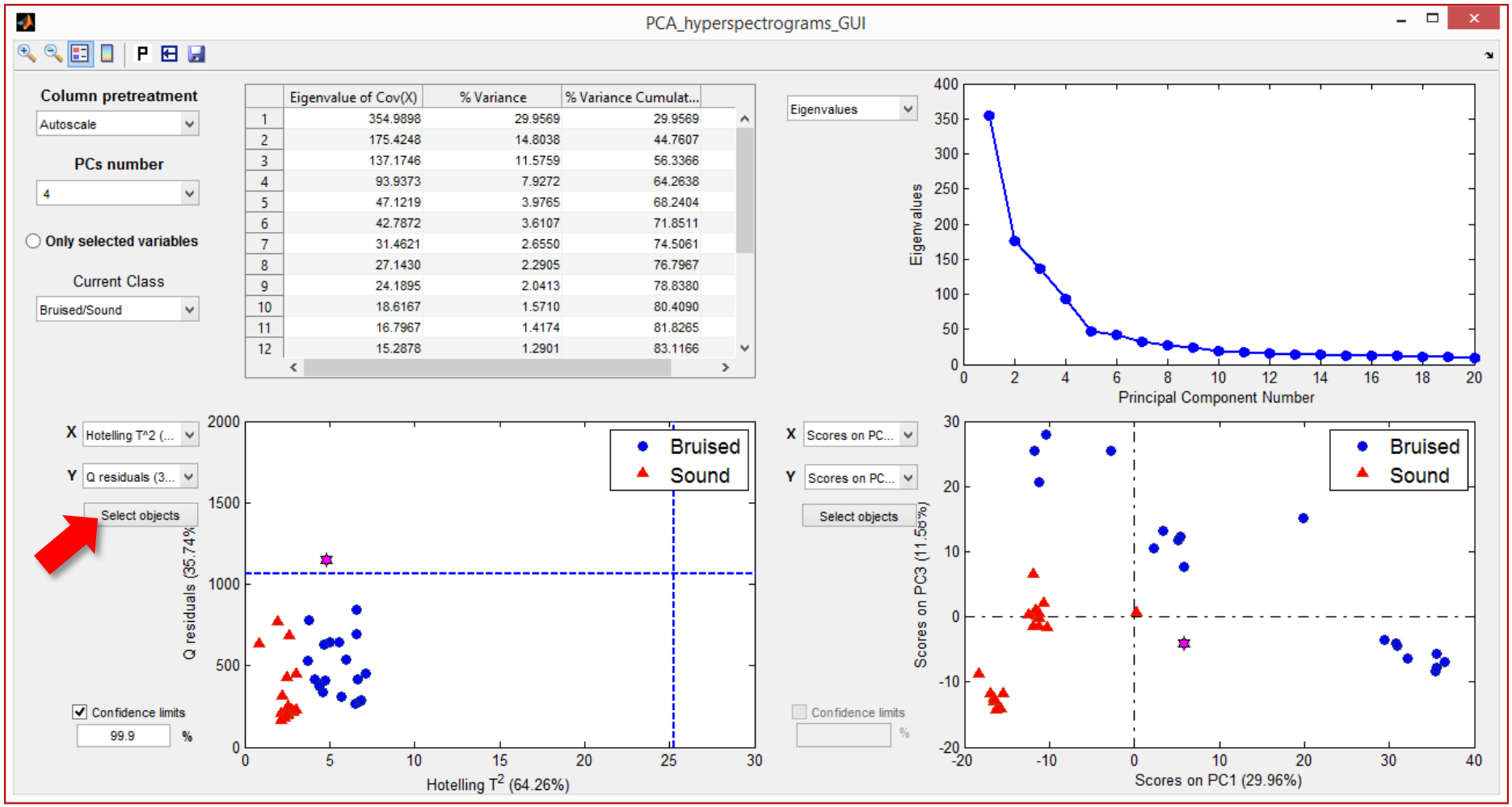
Only Selected Variables

By clicking on the “Only selected variables” radio button a specific window appears, allowing to define the variables to be used for the calculation of the PCA model. Once the included variables are specified, the PCA model is automatically updated



Select objects

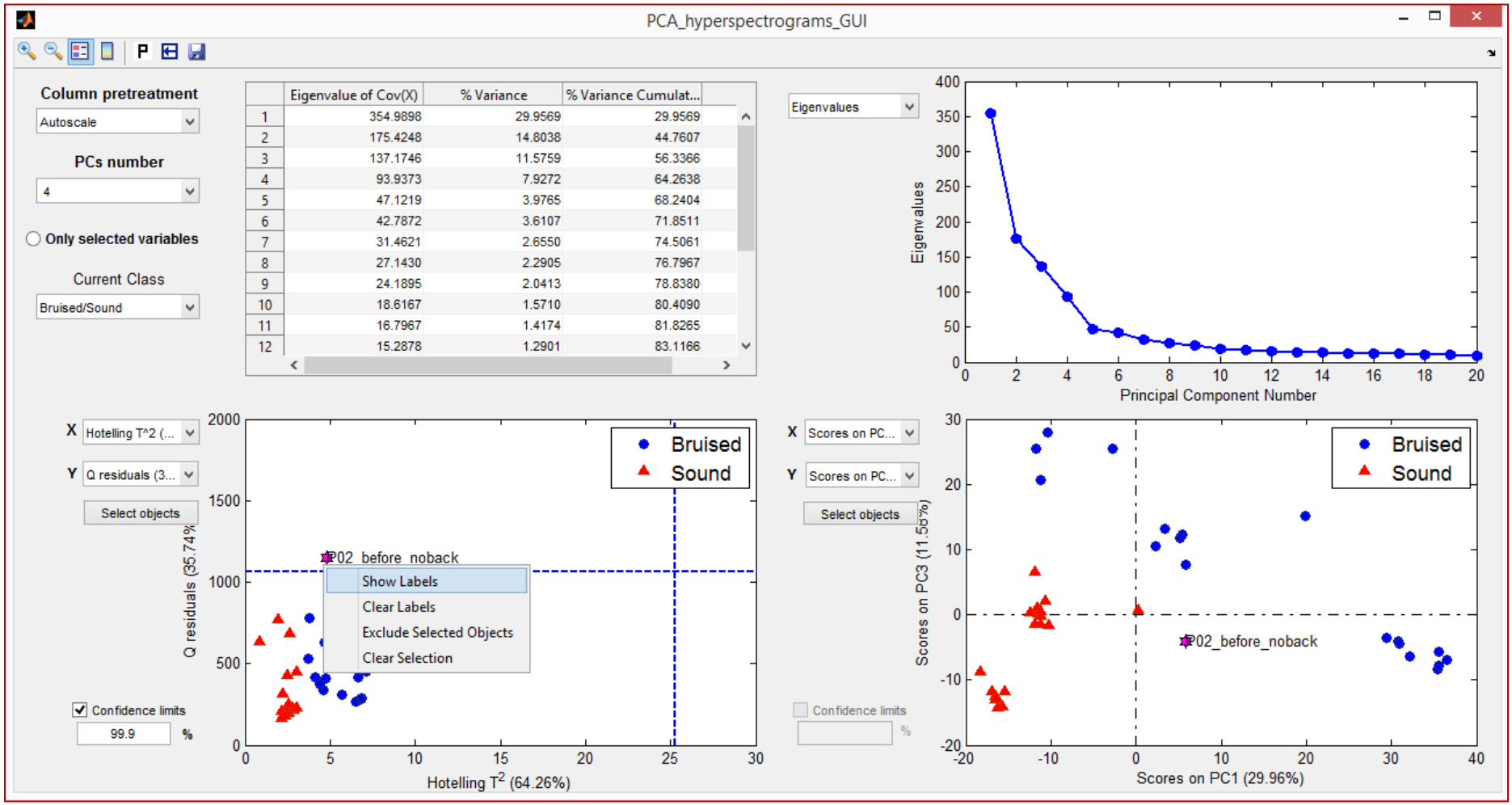
The “Select objects” push buttons associated with Plot 1 and Plot 2 allow to select some objects of interest directly on the plots, for example objects identified as outliers.



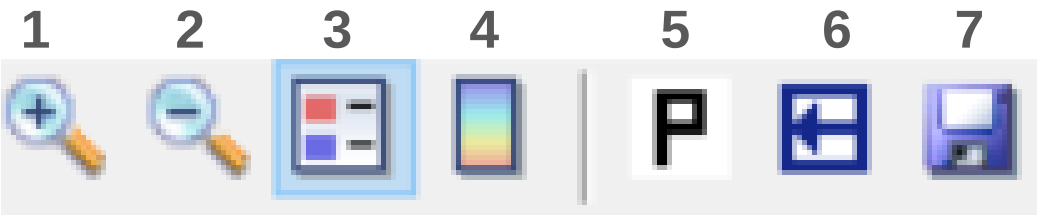
	Eigenvalue of Cov(X)	% Variance	% Variance Cumulat...
1	354.9898	29.9569	29.9569
2	175.4248	14.8038	44.7607
3	137.1746	11.5759	56.3366
4	93.9373	7.9272	64.2638
5	47.1219	3.9765	68.2404
6	42.7872	3.6107	71.8511
7	31.4621	2.6550	74.5061
8	27.1430	2.2905	76.7967
9	24.1895	2.0413	78.8380
10	18.6167	1.5710	80.4090
11	16.7967	1.4174	81.8265
12	15.2878	1.2901	83.1166

Select objects

By right-clicking on the magenta hexagrams and using the resulting context menu, the user can decide whether visualizing the labels of the selected objects, deselecting the objects or eliminating them from the dataset. If the selected objects are eliminated, the PCA model is automatically updated



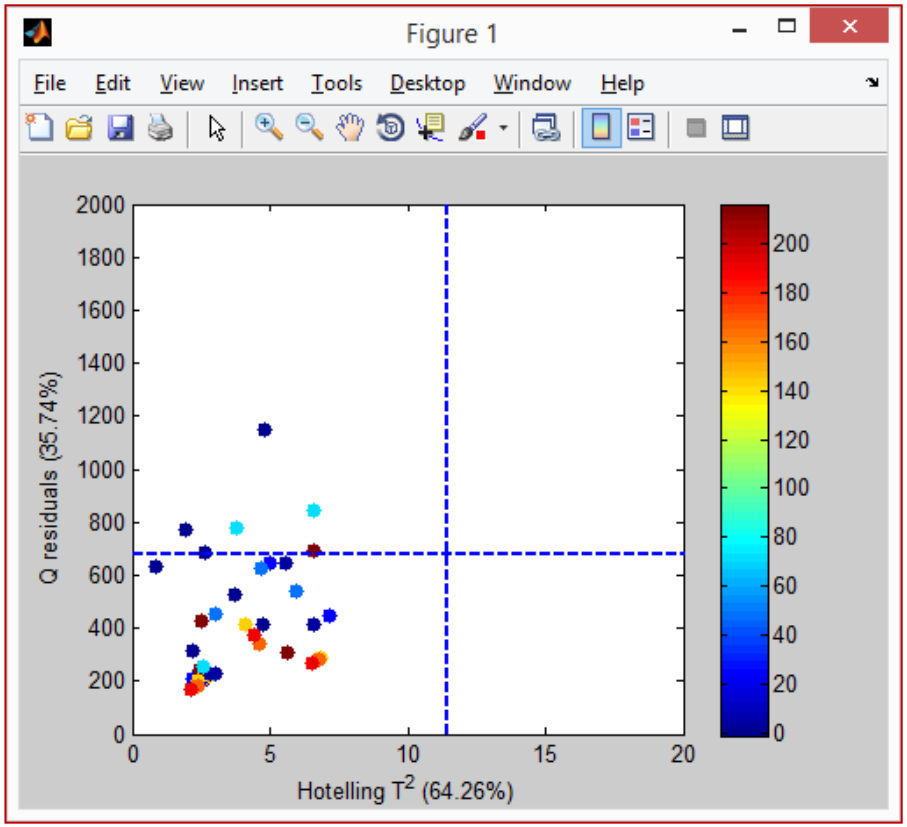
Toolbar – PCA Hyperspectrograms GUI

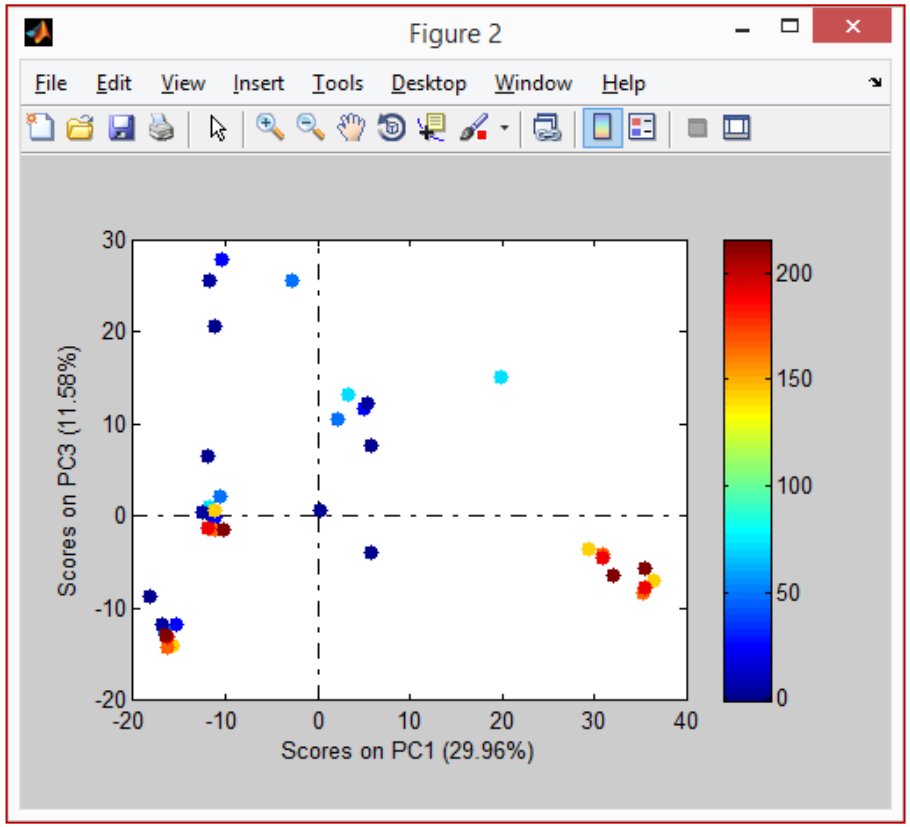


1. Zoom in
2. Zoom out
3. Insert Legend
4. Colour by
5. View Loadings
6. Reinclude samples
7. Save Data

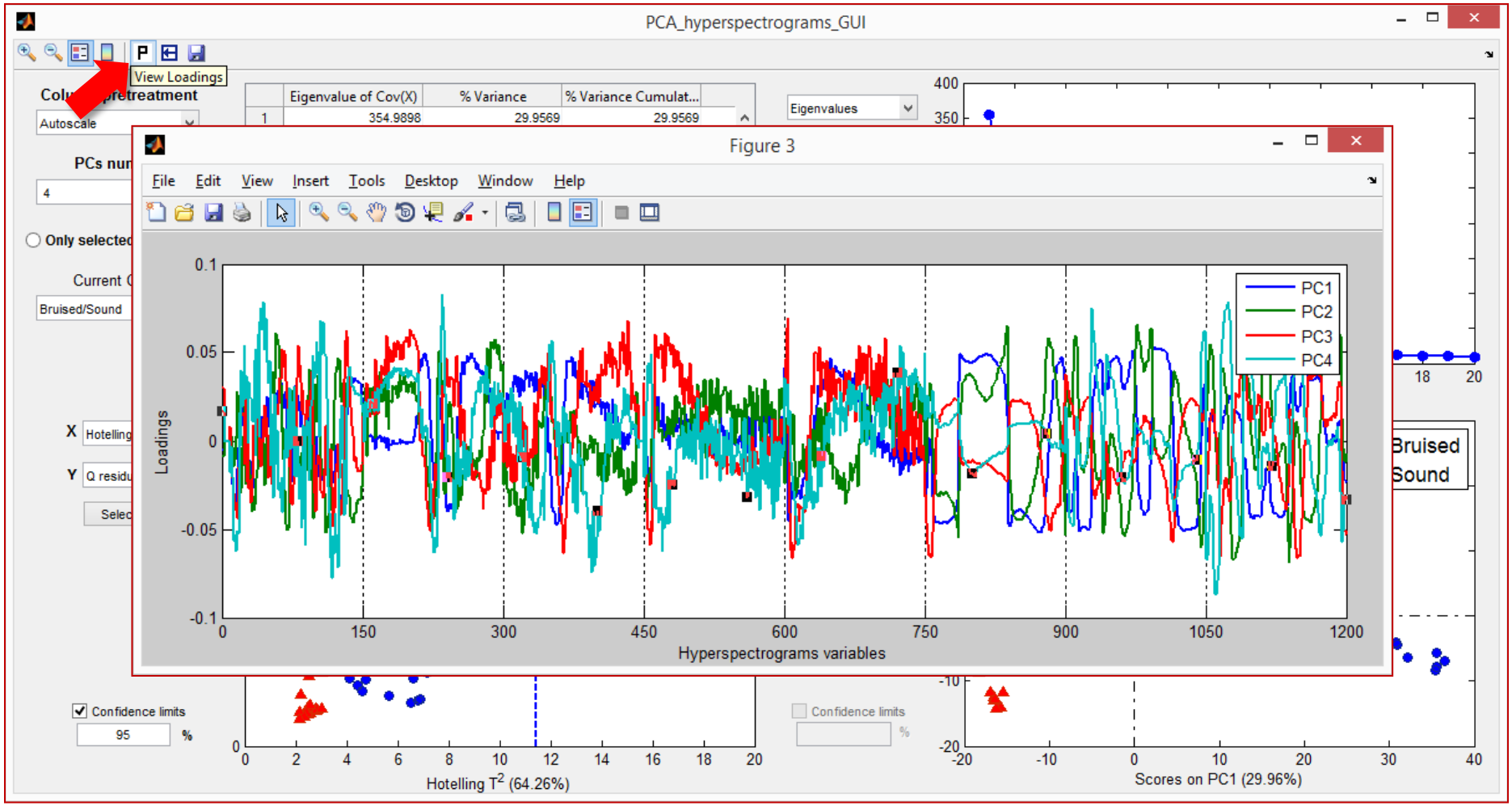
Colour by

The “Colour by” button in the toolbar allows to colour the samples reported in Plot 1 and Plot 2 according to a defined property. This button opens a window to load a vector of numeric values from a MATLAB workspace variable, from a .mat file or from a .xls file. Once the vector has been loaded, two new figures are displayed, one for Plot 1 and one for Plot 2, with the samples coloured according to the chosen property values.





Loading vectors



Save Data

By clicking on the “Save Data” icon, the user can chose whether to save the new (i.e., without the eliminated samples) Dataset or a structure array containing the outputs (scores, loadings, etc..) of the current PCA model.