

### Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix

Select Data

Name of Variable Matrix

Select Variables

Name of Filename Matrix

Select Filenames

Name of Totalcounts Matrix

Select Totalcounts

Name of Samplenames Matrix

Select Samples

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

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Select Samples

This tutorial will provide a general introduction to working with the spectragui.

Please read and follow all tutorials provided for the spectragui.

The tutorials cover each panel and function in the spectragui step by step. This should help you avoid problems or errors.

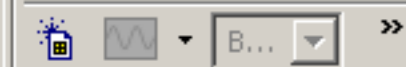
If something doesn't work "as expected" please check the Matlab console for any errors. I have tried hard to catch any possible errors and provide error messages that explain what happened or what you need to do to continue.

If you think something is not working properly or you get an error that outputs to the Matlab workspace, restart the gui and try to re-do what happened when you got the error.

Restarting the spectragui will fix most problems. This is mainly a problem with Matlab getting messed up and not a problem specific to the spectragui.

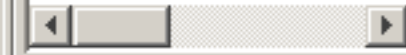
← →

Workspace



Name ▲

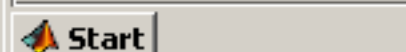
Name ▲
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Current Directory Wor

Command History

----- 8/13/10 9:4



Command Window

&gt;&gt;

&gt;&gt;



To start the spectragui type 'spectragui' at the Matlab command prompt and hit <Enter>



I


**Workspace**

Name

Current Directory

**Command Window**

```
>>  
>> spectragui
```



I

**Command History**

8/13/10 9:4

### Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix

Name of Variable Matrix

Name of Filename Matrix

Name of Totalcounts Matrix

Name of Samplenames Matrix



This is the main window of the spectragui. All of the functions within the spectragui will appear on panels within this window.





These are the menus. They provide access to all of the functions within the spectragui.

The menus are organized by task.



These are the m  
Use the drop d

unless you specify otherwise.  
want to use in your analysis.

Name of Data Matrix  
Select Data

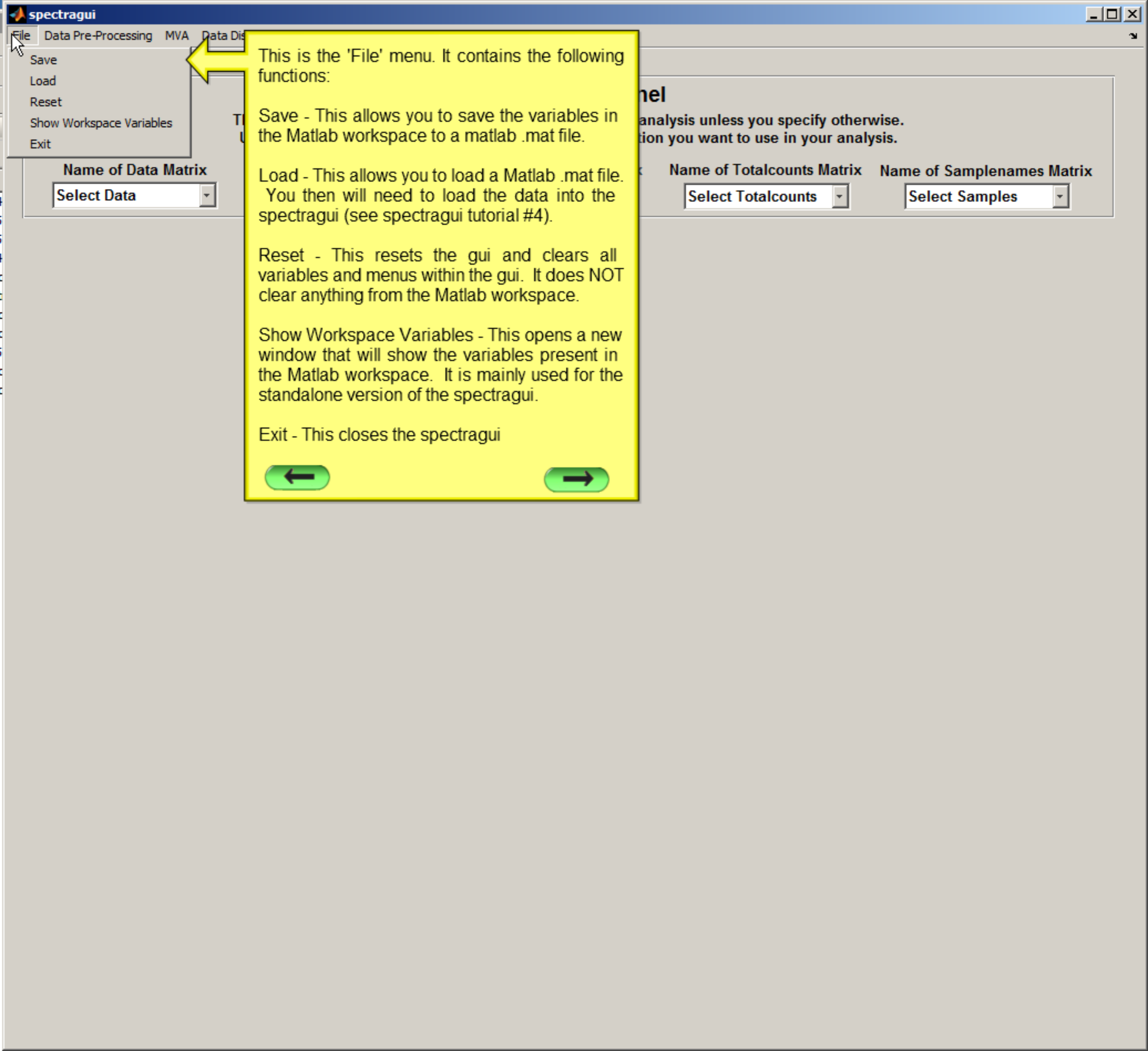
Name of Va  
Select Variables

Select Filenames

e of Totalcounts Matrix  
Select Totalcounts

Name of Samplenames Matrix  
Select Samples





- Save
- Load
- Reset
- Show Workspace Variables
- Exit

This is the 'File' menu. It contains the following functions:

Save - This allows you to save the variables in the Matlab workspace to a matlab .mat file.

Load - This allows you to load a Matlab .mat file. You then will need to load the data into the spectragui (see spectragui tutorial #4).

Reset - This resets the gui and clears all variables and menus within the gui. It does NOT clear anything from the Matlab workspace.

Show Workspace Variables - This opens a new window that will show the variables present in the Matlab workspace. It is mainly used for the standalone version of the spectragui.

Exit - This closes the spectragui



nel

analysis unless you specify otherwise.  
tion you want to use in your analysis.

Name of Totalcounts Matrix

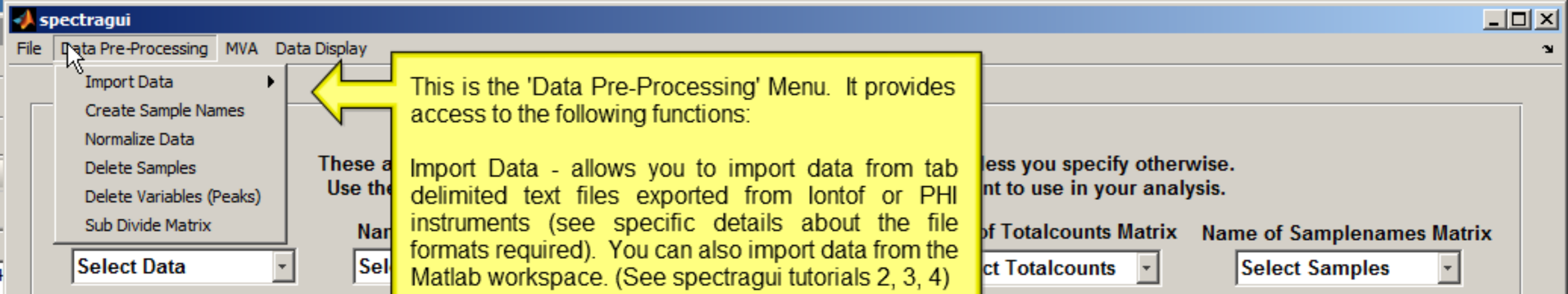
Name of Samplenames Matrix

Select Totalcounts

Select Samples

Name of Data Matrix

Select Data



This is the 'Data Pre-Processing' Menu. It provides access to the following functions:

**Import Data** - allows you to import data from tab delimited text files exported from Iontof or PHI instruments (see specific details about the file formats required). You can also import data from the Matlab workspace. (See spectragui tutorials 2, 3, 4)

**Create Sample Names** - allows you to create a new set of names where each file from a given sample contains the same name. This is required for several functions within the spectragui and must be created to use the spectragui. (See spectragui tutorial 5)

**Normalize Data** - allows you to normalize the data in several ways (See spectragui tutorial 6).

**Delete Samples** - allows you to delete selected files from within a data set. (See spectragui tutorial 11)

**Delete Variables (Peaks)** - allows you to delete variables from a data set. Remember if you normalize to sum of selected peaks and then remove some peaks you must start with the original data and re-normalize to the new peak set. (See spectragui tutorial 12)

**Sub Divide Matrix** - allows you to select a subset of samples or re-order the samples within the data matrix. (See spectragui tutorial 13)





Import Data  
Create Sample Names  
Normalize Data  
Delete Samples  
Delete Variables (Peaks)  
Sub Divide Matrix

Import from Workspace  
IonTof  
Physical Electronics

These are the main input data  
Use the drop down menus to

Name of Variable Matrix  
Select Variables

Select Data

This is the 'Import Data' sub menu showing the choices of data you can import.

The data must be contained within the correct active directory of Matlab and be formatted properly for the scripts to work.

See spectragui tutorials 2, 3, and 4 for more information.

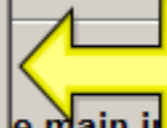
Specify otherwise.  
your analysis.

nts Matrix Name of Samplenames Matrix

nts Select Samples



- Run PCA
- PCA Modelling
- Run DPCA
- Export MVA Data
- Find Correlated Peaks



This is the MVA menu. It provides access to the following functions:

Run PCA - allows you to run PCA on your data. (See spectragui tutorial 7)

PCA Modelling - allows you to load a previously saved PCA model and project new data into the model for classification purposes. (See spectragui tutorial 17)

Run DPCA - allows you to run DPCA as described in Yandle and Macfie in J. Chemometrics, v. 3, p. 589-600 (1989). (See spectragui tutorial 16)

Export MVA Data - allows you to export the scores, loadings, and percent variance data into text files that can be used in other programs. (See spectragui tutorial 10)

Find correlated Peaks - This function finds all peaks that show the same trends with regards to the average relative intensity across the sample set. It can be very useful to help in interpreting PCA results. (See spectragui tutorial 20)



Name of Data Matrix

Select Data

Name of Variable

Select Variables

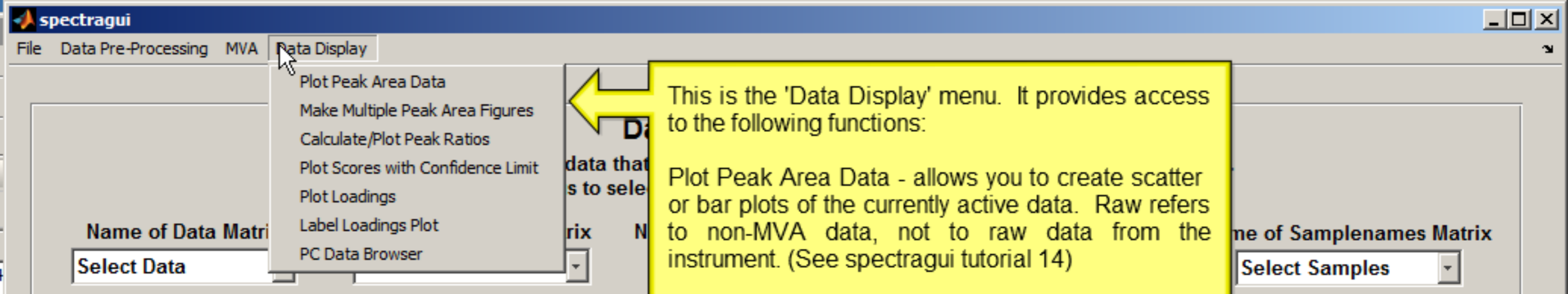
Specify otherwise.  
in your analysis.

Units Matrix

Units

Name of Samplenames Matrix

Select Samples



This is the 'Data Display' menu. It provides access to the following functions:

Plot Peak Area Data - allows you to create scatter or bar plots of the currently active data. Raw refers to non-MVA data, not to raw data from the instrument. (See spectragui tutorial 14)

Make Multiple Peak Area Figures - allows you to create a series of plots automatically. Basically it is an automated version of the 'Plot Raw Data' function. (See spectragui tutorial 15)

Calculate/Plot Peak Ratios - Allows you to calculate and plot peak area ratios from any combination of peaks. (See spectragui tutorial 21)

Plot Scores with Confidence Limit - allows you to plot the scores using the 95% confidence limit as described by Langmuir 17: 4649 (2001). (See spectragui tutorial 08)

Plot Loadings - allows you to plot the loadings for any PC vs m/z. It creates nice looking figures. (See spectragui tutorial 09)

Label Loadings Plot - allows you to label peaks within a loading plot created using the Plot Loadings function. (See spectragui tutorial 09)

PC Data Browser - Allows you to plot peak area data for a given peak after subtracting previous PCs from the data set. (See spectragui tutorial 22)



### Data Selection Panel

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Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
Select Data	Select Variables	Select Filenames	Select Totalcounts	Select Samples

This is the 'Data Selection Panel'. I provides access to the data loaded in the gui.

When using the gui, the drop down menus below are automatically populated with the appropriate data. The data that is shown is the currently active data that will be used in the various functions of the spectragui.

← →

### Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix

Select Data

Select Data

ndatass

Name of Variable Matrix

Select Variables

Name of Filename Matrix

Select Filenames

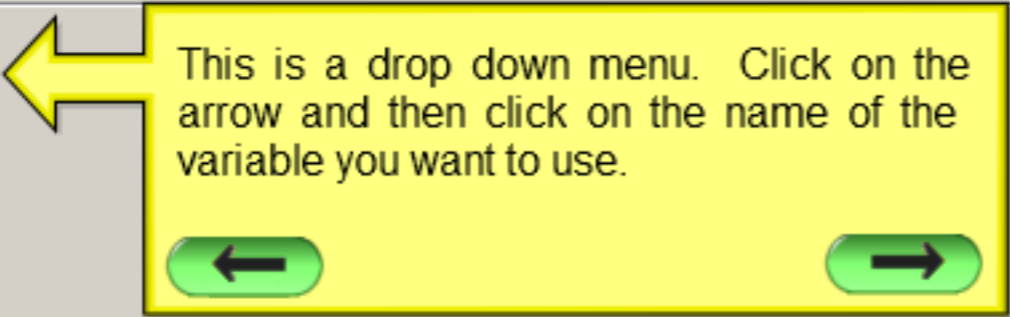
Name of Totalcounts Matrix

Select Totalcounts

Name of Samplenames Matrix

Select Samples

This is a drop down menu. Click on the arrow and then click on the name of the variable you want to use.



### Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix <input type="text" value="Select Data"/>	Name of Variable Matrix <input type="text" value="Select Variables"/>	Name of Filename Matrix <input type="text" value="Select Filenames"/>	Name of Totalcounts Matrix <input type="text" value="Select Totalcounts"/>	Name of Samplenames Matrix <input type="text" value="Select Samples"/>
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### MVA Data Selection Panel

Name of Scores Matrix <input type="text" value="Select Scores"/>	Name of Loadings Matrix <input type="text" value="Select Loadings"/>	Name of % Variance Matrix <input type="text" value="Select %Variance"/>	Name of Model Matrix <input type="text" value="Select Model"/>
---	---	--	---

### Plot Scores

Load Selected Data

Scores:	None
Samples:	None
Variance:	None

This is the MVA Data Selection Panel.

After saving the results from a MVA, the drop down menus in this panel are populated with the respective MVA results.

This panel is only active with functions that require MVA information.

X-Axis      Y-Axis

<input type="text"/>	<input type="text"/>
----------------------	----------------------

Confidence Limit

<input type="button" value="Plot Scores"/>	<input type="button" value="Save Scores Plot"/>
<input type="button" value="Make Ext"/>	<input type="button" value="Close Panel"/>

### Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
Select Data	Select Variables	Select Filenames	Select Totalcounts	Select Samples

### MVA Data Selection Panel

Name of Scores Matrix	Name of Loadings Matrix	Name of % Variance Matrix	Name of Model Matrix
Select Scores	Select Loadings	Select %Variance	Select Model

Select Scores  
newscores

These menus work the same as the drop down menus in the 'Data Selection Panel'

Load Selected Data

Load Selected Data

Scores: None  
Samples: None  
Variance: None

X-Axis

Y-Axis

X-Axis plot area

Y-Axis plot area

Confidence Limit

%

Plot Scores

Save Scores Plot

Make Ext

Close Panel

### Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix <input type="text" value="Select Data"/>	Name of Variable Matrix <input type="text" value="Select Variables"/>	Name of Filename Matrix <input type="text" value="Select Filenames"/>	Name of Totalcounts Matrix <input type="text" value="Select Totalcounts"/>	Name of Samplenames Matrix <input type="text" value="Select Samples"/>
---	--	--	---	---

### MVA Data Selection Panel

Name of Scores Matrix <input type="text" value="Select Scores"/>	Name of Loadings Matrix <input type="text" value="Select Loadings"/>	Name of % Variance Matrix <input type="text" value="Select %Variance"/>	Name of Model Matrix <input type="text" value="Select Model"/>
---	---	--	---

### Plot Scores

Load Selected Data

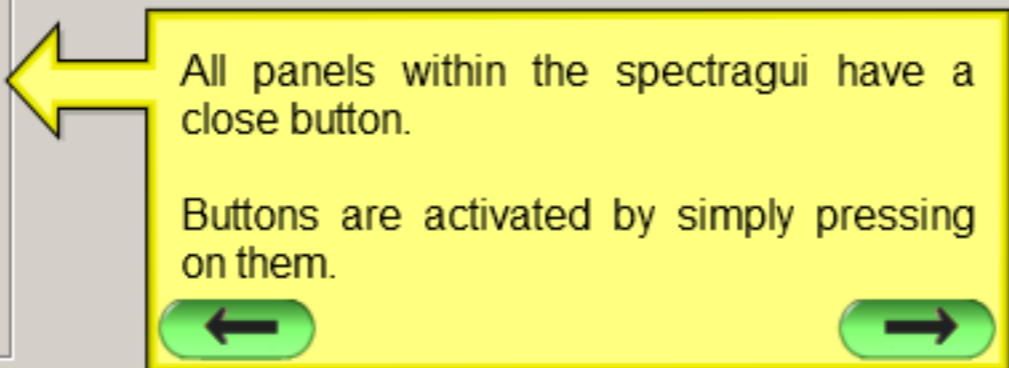
Scores:	None
Samples	None
Variance:	None

X-Axis

Y-Axis

Confidence Limit

<input type="button" value="Plot Scores"/>	<input type="button" value="Save Scores Plot"/>
<input type="button" value="Make Ext"/>	<input type="button" value="Close Panel"/>

 All panels within the spectragui have a close button.  
Buttons are activated by simply pressing on them.



### Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix

Select Data

Name of Variable Matrix

Select Variables

Name of Filename Matrix

Select Filenames

Name of Totalcounts Matrix

Select Totalcounts

Name of Samplenames Matrix

Select Samples

To illustrate a few more basics of using the spectra gui, I will open a panel and load some data.



### Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
Select Data	Select Variables	Select Filenames	Select Totalcounts	Select Samples

Select the data you want to process above and press the "Load Selected Data" button.

Enter a name for the normalized data. Then choose a normalization method and press the 'Normalize' button.

If you choose to normlize by a selected peak, you must select a peak before pressing 'Normalize'.

### Data Normalization

Name for Normalized Matrix

Normalization Method

Normalize

Close Panel

Peak List

Load Selected Data

Data:	None
Variables:	None
Total counts:	None

This box shows what data must be selected in order to use the functions of this panel.

← →

### Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix

Select Data

Select Data  
ndatass

Name of Variable Matrix

Select Variables

Name of Filename Matrix

Select Filenames

Name of Totalcounts Matrix

Select Totalcounts

Name of Samplenames Matrix

Select Samples

Select the data you want by clicking on the down arrow and then clicking on the item you want to select.

Select the data you want to process above and press the "Load Selected Data" button.

Enter a name for the normalized data. Then choose a normalization method and press the 'Normalize' button.

If you choose to normlize by a selected peak, you must select a peak before pressing 'Normalize'.

Normalization Method

Choose an option b...

Normalize

Close Panel

Peak List

Load Selected Data

Data:	None
Variables:	None
Total counts:	None

### Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix

ndatass

Name of Variable Matrix

Select Variables

Name of Filename Matrix

Select Filenames

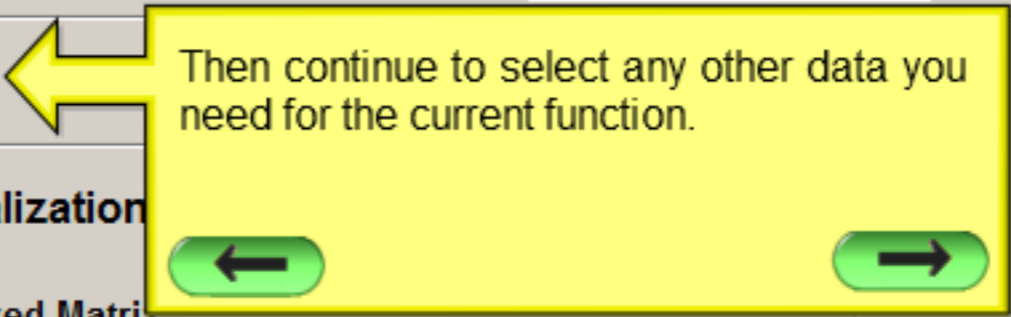
Name of Totalcounts Matrix

Select Totalcounts

Name of Samplenames Matrix

Select Samples

Then continue to select any other data you need for the current function.



Select the data you want to process above and press the "Load Selected Data" button.

Enter a name for the normalized data. Then choose a normalization method and press the 'Normalize' button.

If you choose to normlize by a selected peak, you must select a peak before pressing 'Normalize'.

### Data Normalization

Name for Normalized Matrix

Normalization Method

Choose an option b...

Normalize

Close Panel

Load Selected Data

Data:	None
Variables:	None
Total counts:	None

### Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
<input type="text" value="ndatass"/>	<input type="text" value="exactmass"/>	<input type="text" value="Select Filenames"/>	<input type="text" value="totalcounts"/>	<input type="text" value="Select Samples"/>

Select the data you want to process above and press the "Load Selected Data" button.

Enter a name for the normalized data. Then choose a normalization method and press the 'Normalize' button.

If you choose to normlize by a selected peak, you must select a peak before pressing 'Normalize'.

### Data Normalization

Name for Normalized Matrix

Normalization Method

Peak List

Data:	None
Variables:	None
Total counts:	None

Once the required data is selected from the 'Data Selection Panel' press the 'Load Selected Data' button to read the data into the current panel.



### Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
<input type="text" value="ndatass"/>	<input type="text" value="exactmass"/>	<input type="text" value="Select Filenames"/>	<input type="text" value="totalcounts"/>	<input type="text" value="Select Samples"/>

Select the data you want to process above and press the "Load Selected Data" button.

Enter a name for the normalized data. Then choose a normalization method and press the 'Normalize' button.

If you choose to normlize by a selected peak, you must select a peak before pressing 'Normalize'.

### Data Normalization

Name for Normalized Matrix

Normalization Method

Normalize

Close Panel

### Peak List

- 11.9999
- 13.0080
- 14.0162
- 15.9963
- 17.0030
- 24.0008
- 25.0078
- 31.9726
- 32.9796
- 34.9757
- 36.0015
- 37.0086
- 38.0166
- 39.0212

Load Selected Data

Data: **ndatass**  
Variables: **exactmass**  
Total counts: **totalcounts**

The loaded data is highlighted in red.

← →

### Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix  
ndatass

Name of Variable Matrix  
exactmass

Name of Filename Matrix  
Select Filenames

Name of Totalcounts Matrix  
totalcounts

Name of Samplenames Matrix  
Select Samples

I have spent a lot of time trying to make sure that the spectragui will notify you when you make a mistake.

This is done by a pop-up error message that will describe what you did wrong or how to correct it.

← →



### Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix

ndatass

Select Data

ndatass

Name of Variable Matrix

exactmass

Name of Filename Matrix

Select Filenames

Name of Totalcounts Matrix

totalcounts

Name of Samplenames Matrix

Select Samples

For example if we select the menu title instead of a menu item an error is output.





### Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix

Select Data

Name of Variable Matrix

exactmass

Name of Filename Matrix

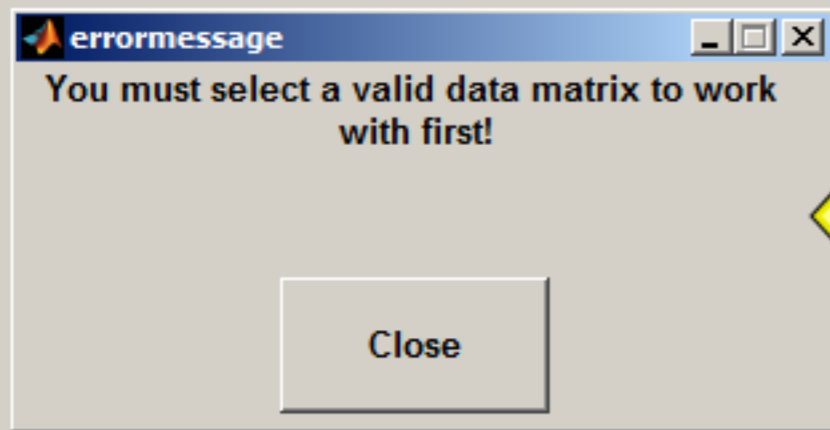
Select Filenames

Name of Totalcounts Matrix

totalcounts

Name of Samplenames Matrix

Select Samples



This is the error message box. It describes what went wrong and suggests how to fix the problem.

Press 'Close' to close the box. If you don't close it you will end up with multiple error message boxes open if you make another mistake.

← →

### Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix

Select Data

Name of Variable Matrix

exactmass

Name of Filename Matrix

Select Filenames

Name of Totalcounts Matrix

totalcounts

Name of Samplenames Matrix

Select Samples

That's it for a general overview of the spectragui.

Continue on to another tutorial to learn how to use specific panels/functions within the gui.

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.

