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.
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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.
To start the spectragui type 'spectragui' at the Matlab command prompt and hit <Enter>
>>
>> spectragui
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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.
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
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)
This is the 'Import Data' sub menu showing the choices of data you can import.

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

See spectragui tutorials 2, 3, and 4 for more information.
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)
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)
This is the 'Data Selection Panel'. It 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.

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

MVA Data Selection Panel

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

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<th>Name of Total counts Matrix</th>
<th>Name of Sample names Matrix</th>
</tr>
</thead>
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<td>Select Variables</td>
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<td>Select Total counts</td>
<td>Select Samples</td>
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</table>

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 normalize by a selected peak, you must select a peak before pressing 'Normalize'.

Data Normalization

Name for Normalized Matrix

Normalization Method

Load Selected Data

Normalize

Close Panel

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.

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

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

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 normalize by a selected peak, you must select a peak before pressing 'Normalize'.

Data Normalization

Name for Normalized Matrix
Normalization Method

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: 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: exactmass
Name of Filename Matrix: Select Filenames
Name of Totalcounts Matrix: totalcounts
Name of Samplenames Matrix: 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 normalize by a selected peak, you must select a peak before pressing 'Normalize'.

The loaded data is highlighted in red.
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.

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<td>select</td>
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For example, if we select the menu title instead of a menu item, an error is output.
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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.
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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.