

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

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.

Workspace

Name

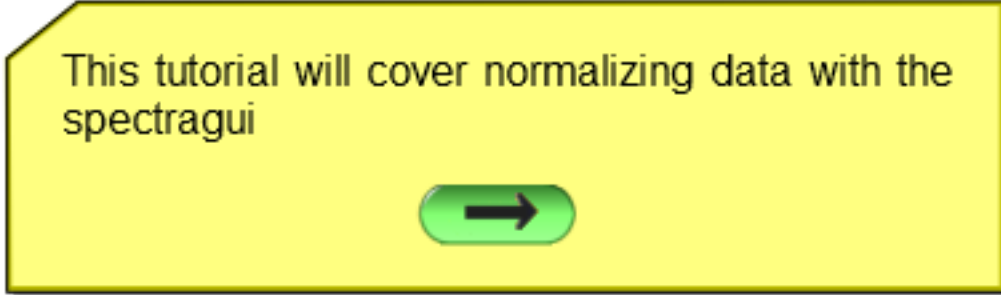
Current Directory Wor

Command Window

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I

This tutorial will cover normalizing data with the spectragui



Command History

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Workspace

Name

- data
- exactmass
- filenames
- labels
- nommass
- samplenames
- totalcounts

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Command History

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>> spectragui
  
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From the 'Data Pre-Processing' menu choose -> 'Normalize Data'



These a

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analysis unless you specify otherwise

Name of Data Matrix Name of Totalcounts Matrix Name of Samplenames Matrix

Select Data Select Variables filenames Select Totalcounts Select Samples



Workspace

Name

- data
- exactmass
- filenames
- labels
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- samplenames
- totalcounts

Current Directory

Command History

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>> spectragui

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Raw Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise

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

Select the data to be processed and the normalization method. Enter a name for the data. The normalization method and press the 'Normalize' button.

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

Choose an option ...

Normalize

Load Selected Data

Close Panel

Peak List

Data: None
Variables: None
Total counts: None

Make sure the correct data and other variables are selected from the drop down menus in the 'Raw Data Selection Panel'



Workspace

Name
data
exactmass
filenames
labels
nommass
samplenames
totalcounts

Current Directory

Command History

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>> spectragui
  
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Raw Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
data	exactmass	filenames	totalcounts	samplenames

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

Normalize

Peak List

Load Selected Data

Press the 'Load Selected Data' button

Data:	None
Variables:	None
Total counts:	None



Workspace

Name
data
exactmass
filenames
labels
nommass
samplenames
totalcounts

Current Directory

Command History

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>> spectragui
  
```

Raw Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
data	exactmass	filenames	totalcounts	samplenames

Data Normalization

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 presssing 'Normalize'.

Name for Normalized Matrix:

Normalization Method: Choose an option ...

Peak List: 12, 13, 14, 16, 17, 24, 25, 32, 33, 35, 36, 37, 38

Buttons: Load Selected Data, Normalize, Close Panel

Summary: Data: data, Variables: exactmass, Total counts: totalcounts

The GUI highlights what data is being used within the given panel.

The list of selected peaks is shown here. This list can be used to normalize the data to a selected peak.

Workspace

Name

- data
- exactmass
- filenames
- labels
- nommass
- samplenames
- totalcounts

Current Directory

Command History

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Raw Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
data	exactmass	filenames	totalcounts	samplenames

Data Normalization

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.

Name for Normalized Matrix

Normalization Method

Choose an option

Peak List

- 12
- 13
- 14
- 16
- 17
- 24
- 25
- 32
- 33
- 35
- 36
- 37
- 38

Enter a name for the normalized data. This can be any name you want, but should be descriptive of how you normalize the data.

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Close Panel

Data:	data
Variables:	exactmass
Total counts:	totalcounts

Workspace

Name

- data
- exactmass
- filenames
- labels
- nommass
- samplenames
- totalcounts

Current Directory

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Raw Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
data	exactmass	filenames	totalcounts	samplenames

Data Normalization

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'

Name for Normalized Matrix

Normalization Method

Peak List

- 12
- 13
- 14
- 16
- 17
- 24
- 25
- 32
- 33
- 35
- 36
- 37
- 38

Normalize

Choose how you want to normalize the data from the drop down menu.

Variables: **exactmass**

Total counts: **totalcounts**

Workspace

Name
data
exactmass
filenames
labels
nommass
samplenames
totalcounts

Current Directory

Command History

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Raw Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
data	exactmass	filenames	totalcounts	samplenames

Data Normalization

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'.

Name for Normalized Matrix

Normalization Method
 Choose an option ...
 Choose an option below
 Sum of selected peaks
 Largest peak in spectrum
 User selected peak
 Total intensity of spectrum

Peak List

12
13
14
16
17
24
25
32
33
35
36
37
38

Buttons: Load Selected Data, Normalize

Callout: In this case, I am choosing to use the sum of selected peaks.

Workspace

Name
data
exactmass
filenames
labels
nommass
samplenames
totalcounts

Command History

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>>
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Current Directory

Raw Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
data	exactmass	filenames	totalcounts	samplenames

Data Normalization

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'.

Name for Normalized Matrix:

Normalization Method:

Peak List:

12
13
14
16
17
24
25
32
33
35
36
38

Buttons: Load Selected Data, Normalize, Close Panel

Note: this button to normalize your data.

Instruction Box: Now press the 'Normalize' button.



Workspace

Name

- data
- exactmass
- filenames
- labels
- ndatass
- nommass
- samplenames
- totalcounts

Current Directory

Command History

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Raw Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
data	exactmass	filenames	totalcounts	samplenames

Data Normalization

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'.

Name for Normalized Matrix:

Normalization Method:

Peak List

- 12
- 13
- 14
- 16
- 17
- 24
- 25
- 32
- 33
- 35
- 36
- 37
- 38

Your normalized data is now ready

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

A message confirms that the data has been normalized.

The normalized data is added to the 'Data Matrix' drop down menu in the 'Raw Data Selection Panel' and to the Matlab workspace.

Workspace

Name

- data
- exactmass
- filenames
- labels
- indatass
- nommass
- samplenames
- totalcounts

Command Window

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The new data was created and saved to the Matlab workspace.

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spectragui
```

of Samplenames Matrix
samplenames



Workspace

Name

- data
- exactmass
- filenames
- labels
- ndatass
- nommass
- samplenames
- totalcounts

Current Directory

Command History

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>> spectragui
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Raw Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise

Name of Data Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

Make sure the correct data is selected before you proceed to further analysis.

In this case, I want to use the normalized data I just created.

← →



Workspace

Name

- data
- exactmass
- filenames
- labels
- ndatass
- nommass
- samplenames
- totalcounts

Current Directory

Command History

```
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Raw Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise

Name of Data Matrix	Name of Variable Matrix	Name of Filename Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
ndatass	exactmass	filenames	totalcounts	samplenames

That's it for this tutorial.

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.

