

### 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.

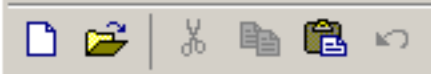


This is the 'Go to URL' button. It takes you to a website link.



Press the 'Next' button below to start this tutorial.





Shortcuts How to Add

Workspace



Name

- data
- exactmass
- filenames
- i
- newdata
- newfiles
- newsamples
- nommass
- peaklabels
- peakstoplot
- samplenames
- totalcounts



Current Directory Workspace

Command History

```

-- 10/6/10 3:44
- peakstoplot
- peaklables
- clc
- peakstoplot
- peaklabels

```

### 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
data	exactmass	filenames	totalcounts	samplenames

This tutorial will cover how to generate multiple raw data figures automatically using the 'Make Multiple Peak Area Figures' function.

This function allows you to quickly make peak area figures from a large number of peaks.

← →

- Plot Peak Area Data
- Make Multiple Peak Area Figures**
- Calculate/Plot Peak Ratios
- Plot Scores with Confidence Limit
- Plot Loadings
- Label Loadings Plot
- PC Data Browser

From the 'Data Display' menu choose -> 'Make Multiple Peak Area Figures'

Name of Data Matrix  
Select Data

Select Filenames

Select Totalcounts

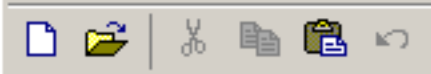
Name of Samplenames Matrix  
Select Samples

data that  
s to sele

otherwise.  
r analysis.

rix

matrix



Shortcuts How to Add

Workspace



Name

- data
- exactmass
- filenames
- i
- newdata
- newfiles
- newsamples
- nommass
- peaklabels
- peakstoplot
- samplenames
- totalcounts

Current Directory Workspace

Command History

```

-- 10/6/10 3:44
peakstoplot
peaklables
clc
peakstoplot
peaklabels

```

### 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:

### Make Multiple Raw Data Figures Panel

Choose the data and samplenames you want to work with in the 'Load Selected' panel

Make sure the data you want to plot is selected in the 'Data Selection Panel'

← →

Name of Selected Variables

Name of Peak Labels

Load Selected

List of selected Peaks

Output Filename List

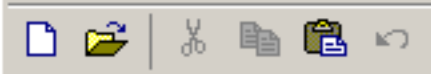
Select Plot Type

Select Figure Output Format

Generate Figure names

Make Figures

Close Panel



Shortcuts How to Add

Workspace

- Name
- data
- exactmass
- filenames
- i
- newdata
- newfiles
- newsamples
- nommass
- peaklabels
- peakstoplot
- samplenames
- totalcounts

Current Directory Workspace

Command History

```

-- 10/6/10 3:44
peakstoplot
peaklables
clc
peakstoplot
peaklabels

```

### 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:

### Make Multiple Raw Data Figures Panel

Choose the data, variables and samplenames you want to work with and press the 'Load Selected' button.

Currently Loaded  
Data: None  
Variables: None

Name of Selected Variables:

Name of Peak Labels:

Load Selected

List of selected Peaks:

List of selected Peaks:

Select Plot Type:

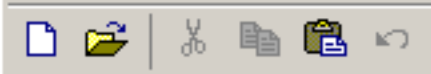
Select Figure Output Format:

Generate Figure names

Make Figures

Close Panel

Press the 'Load Selected' Button



Shortcuts How to Add

Workspace

- Name
- data
- exactmass
- filenames
- i
- newdata
- newfiles
- newsamples
- nommass
- peaklabels
- peakstoplot
- samplenames
- totalcounts

Current Directory Workspace

Command History

```

-- 10/6/10 3:44
peakstoplot
peaklables
clc
peakstoplot
peaklabels

```

### 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="data"/>	Name of Variable Matrix <input type="text" value="exactmass"/>	Name of Filename Matrix <input type="text" value="filenames"/>	Name of Totalcounts Matrix <input type="text" value="totalcounts"/>	Name of Samplenames Matrix <input type="text" value="samplenames"/>
--	---	---	--	--

### Make Multiple Raw Data Figures Panel

Choose the data, variables and samplenames you want to work with and press the 'Load Selected' button.

Load Selected

**Currently Loaded**

Data: **data**  
 Variables: **exactmass**  
 Samplenames: **samplenames**

Name of Selected Variables

The selected data is loaded into the current gui panel.

← →

**List of selected Peaks**

**Output Filename List**

Generate Figure names

Select Plot Type

Choose Plot Type

Select Figure Output Format

Choose Output Format

Make Figures

Close Panel

Workspace

Name	Value
data	<42x84 double>
exactmass	<84x15 char>
filenames	<42x15 char>
i	10
newdata	<36x84 double>
newfiles	<36x15 char>
newsamples	<36x4 char>
nommass	<84x15 char>
peaklabels	<7x3 char>
peakstoplot	<7x15 char>
samplenames	<42x4 char>
totalcounts	<42x1 double>

Current Directory Workspace

Command History

```
-- 10/6/10 3:44 PM --%  
peakstoplot  
peaklables  
clc  
peakstoplot  
peaklabels  
clc
```

Command Window

```
>> p|
```

Before we continue, we need to have a variable in our Matlab workspace that has which peaks we want to create figures for and a variable that contains the labels we want to use in the plots.

I created some example variables for this tutorial called 'peakstoplot' and 'peaklabels'



Name	Value
data	<42x84 double>
exactmass	<84x15 char>
filenames	<42x15 char>
i	10
newdata	<36x84 double>
newfiles	<36x15 char>
newsamples	<36x4 char>
nommass	<84x15 char>
peaklabels	<7x3 char>
peakstoplot	<7x15 char>
samplenames	<42x4 char>
totalcounts	<42x1 double>

Current Directory Workspace

Command History
%-- 10/6/10 3:44 PM --%
peakstoplot
peaklables
clc
peakstoplot
peaklabels
clc
peakstoplot
peaklabels

```
>> peakstoplot

peakstoplot =

11.9999
13.0080
14.0162
15.9963
17.0030
24.0008
25.0078

>> peaklabels

peaklabels =

C
CH
CH2
CH3
O
OH
C2H

>> |
```

You must have a label for each peak you want to plot.

Remember that in Matlab, text labels held within a variable must have the same number of characters. You can use spaces to compensate for labels with different numbers of characters.





Shortcuts How to Add

Workspace

- Name
- data
- exactmass
- filenames
- i
- newdata
- newfiles
- newsamples
- nommass
- peaklabels
- peakstoplot
- samplenames
- totalcounts

Current Directory Workspace

Command History

```

-- 10/6/10 3:44
peakstoplot
peaklables
clc
peakstoplot
peaklabels
clc
peakstoplot
peaklabels

```

### 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:

### Make Multiple Raw Data Figures Panel

Choose the data, variables and samplenames you want to work with and press the 'Load Selected' button

Load Selected

Now enter the name of the variable that has the peaks you want to plot here.

← →

Name of Selected Variables:

Name of Peak Labels:

List of selected Peaks

Output Filename List

Generate Figure names

Select Plot Type

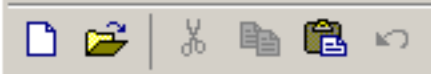
Choose Plot Type

Select Figure Output Format

Choose Output Format

Make Figures

Close Panel



Shortcuts How to Add

Workspace



Name

- data
- exactmass
- filenames
- i
- newdata
- newfiles
- newsamples
- nommass
- peaklabels
- peakstoplot
- samplenames
- totalcounts

Current Directory Workspace

Command History

```

> %-- 10/6/10 3:44
peakstoplot
peaklables
clc
peakstoplot
peaklabels
clc
peakstoplot
peaklabels

```

### 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:

### Make Multiple Raw Data Figures Panel

Choose the data, variables and samplenames you want to work with and press the 'Load Selected' button.

Load Selected

**Currently Loaded**

Data: **data**  
 Variables: **exactmass**  
 Samplenames: **samplenames**

Name of Selected Variables

Name of Peak Labels

#### List of selected Peaks

- 11.9999
- 13.0080
- 14.0162
- 15.9963
- 17.0030
- 24.0008
- 25.0078

#### Output Filename List

- 

The list of selected peaks is automatically populated.

Select Plot Type

Select Figure Output Format

Generate Figure names

Make Figures

Close Panel



Shortcuts How to Add

Workspace

- Name
- data
- exactmass
- filenames
- i
- newdata
- newfiles
- newsamples
- nommass
- peaklabels
- peakstoplot
- samplenames
- totalcounts

Current Directory Workspace

Command History

```

> %-- 10/6/10 3:44
> peakstoplot
> peaklables
> clc
> peakstoplot
> peaklabels
> clc
> peakstoplot
> peaklabels
  
```

### 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:

### Make Multiple Raw Data Figures Panel

Choose the data, variables and samplenames you want to work with and press the 'Load Selected' button.

Currently Loaded  
Data:

**Now enter the name of the variable that has the peak labels you want to use here.**

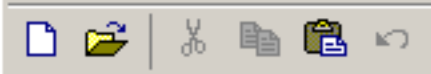
Name of Selected Variables:

Name of Peak Labels:

List of selected Peaks:   
13.0080  
14.0162  
15.9963  
17.0030  
24.0008  
25.0078

Select Plot Type:

Select Figure Output Format:



Shortcuts How to Add

Workspace

- Name
- data
- exactmass
- filenames
- i
- newdata
- newfiles
- newsamples
- nommass
- peaklabels
- peakstoplot
- samplenames
- totalcounts

Current Directory Workspace

Command History

```

-- 10/6/10 3:44
peakstoplot
peaklables
clc
peakstoplot
peaklabels
clc
peakstoplot
peaklabels

```

### 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:

### Make Multiple Raw Data Figures Panel

Choose the data, variables and samplenames you want to work with and press the 'Load Selected' button.

**Currently Loaded**

Data: data

Variables: exactmass

Samplenames: samplenames

Name of Selected Variables:

Name of Peak Labels:

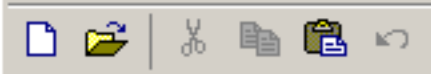
List of selected Peaks:   
 13.0080  
 14.0162  
 15.9963  
 17.0030  
 24.0008  
 25.0078

Output Filename List:

Select Plot Type:

Select Figure Output Format:

Then press the 'Generate Figure names' button.



Shortcuts How to Add

Workspace



Name

- data
- exactmass
- filenames
- i
- newdata
- newfiles
- newsamples
- nommass
- peaklabels
- peakstoplot
- samplenames
- totalcounts

Current Directory Workspace

Command History

```

-- 10/6/10 3:44
peakstoplot
peaklables
clc
peakstoplot
peaklabels
clc
peakstoplot
peaklabels

```

### 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:

### Make Multiple Raw Data Figures Panel

Choose the data, variables and samplenames you want to work with and press the 'Load Selected' button.

**Currently Loaded**

Data: **data**

Variables: **exactmass**

Samplenames: **samplenames**

Name of Selected Variables:

Name of Peak Labels:

**List of selected Peaks**

- 11.9999
- 13.0080
- 14.0162
- 15.9963
- 17.0030
- 24.0008
- 25.0078

**Output Filename List**

- 11\_9999\_C
- 13\_0080\_CH
- 14\_0162\_CH2
- 15\_9963\_CH3
- 17\_0030\_O
- 24\_0008\_OH
- 25\_0078\_C2H

The 'Output Filename List' is populated with the names to be used for the files.

The names consist of the masses of the peaks and the peak labels. Decimal points are replaced by underscores to avoid issues with filename errors.

← →





Shortcuts How to Add

Workspace

- Name
- data
- exactmass
- filenames
- i
- newdata
- newfiles
- newsamples
- nommass
- peaklabels
- peakstoplot
- samplenames
- totalcounts

Current Directory Workspace

Command History

```

-- 10/6/10 3:44
peakstoplot
peaklables
clc
peakstoplot
peaklabels
clc
peakstoplot
peaklabels

```

### 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:

### Make Multiple Raw Data Figures Panel

Choose the data, variables and samplenames you want to work with and press the 'Load Selected' button.

**Load Selected**

**Currently Loaded**

Data: **data**  
 Variables: **exactmass**  
 Samplenames: **samplenames**

Name of Selected Variables:   
 Name of Peak Labels:

List of selected Peaks:   
 Output Filename List:

Select Plot Type:   
 Select Figure Output Format:

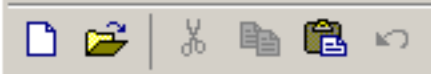
**Make Figures**

**Close Panel**

Choose the type of plot you would like to create.

The same options are available here as in the 'Plot Raw Data' panel (scatter, bar, bar with average and standard deviation, bar with average and standard deviation colored).





Shortcuts How to Add

Workspace

- Name
- data
- exactmass
- filenames
- i
- newdata
- newfiles
- newsamples
- nommass
- peaklabels
- peakstoplot
- samplenames
- totalcounts

Current Directory Workspace

Command History

```

-- 10/6/10 3:44
peakstoplot
peaklables
clc
peakstoplot
peaklabels
clc
peakstoplot
peaklabels

```

### 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:

### Make Multiple Raw Data Figures Panel

Choose the data, variables and samplenames you want to work with and press the 'Load Selected' button.

**Currently Loaded**

Data: data

Variables: exactmass

Samplenames: samplenames

Name of Selected Variables:

Name of Peak Labels:

**List of selected Peaks**

- 11.9999
- 13.0080
- 14.0162
- 15.9963
- 17.0030
- 24.0008
- 25.0078

**Output Filename List**

- 11\_9999\_C
- 13\_0080\_CH
- 14\_0162\_CH2
- 15\_9963\_CH3
- 17\_0030\_O
- 24\_0008\_OH

Select Plot Type:

Select Figure Output Format:

Choose the file format you want to save the files in.

You can choose from '.emf', '.eps', '.jpg', or '.tif'







Shortcuts How to Add

Workspace

- Name
- data
- exactmass
- filenames
- i
- newdata
- newfiles
- newsamples
- nommass
- peaklabels
- peakstoplot
- samplenames
- totalcounts

Current Directory Workspace

Command History

```

> %-- 10/6/10 3:44
> peakstoplot
> peaklables
> clc
> peakstoplot
> peaklabels
> clc
> peakstoplot
> peaklabels

```

### 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:

### Make Multiple Raw Data Figures Panel

Choose the data, variables and samplenames you want to work with and press the 'Load Selected' button.

**Load Selected**

**Currently Loaded**

Data: data

Variables: exactmass

Samplenames: samplenames

**Name of Selected Variables:**

**Name of Peak Labels:**

**List of selected Peaks:**

- 11.9999
- 13.0080
- 14.0162
- 15.9963
- 17.0030
- 24.0008
- 25.0078

**Output Filename List:**

- 11\_9999\_C
- 13\_0080\_CH
- 14\_0162\_CH2
- 15\_9963\_CH3
- 17\_0030\_O
- 24\_0008\_OH
- 25\_0078\_C2H

**Select Plot Type:**

**Select Figure Output Format:**

**Generate Figure names**

Press the 'Make Figures' button.

The figures will be shown rapidly and close as they are saved.

The files are saved to the currently active directory in Matlab (typically the 'work' directory).

The figures will appear and disappear as they are created and saved. When no more figures appear the script is done.



Name of Data Matrix

These Use

ables you

want to work with and press

the 'Load Selected' button.

Load Selected

List of selected Peaks

- 11.9999
- 13.0080
- 14.0162
- 15.9963
- 17.0030
- 24.0008
- 25.0078

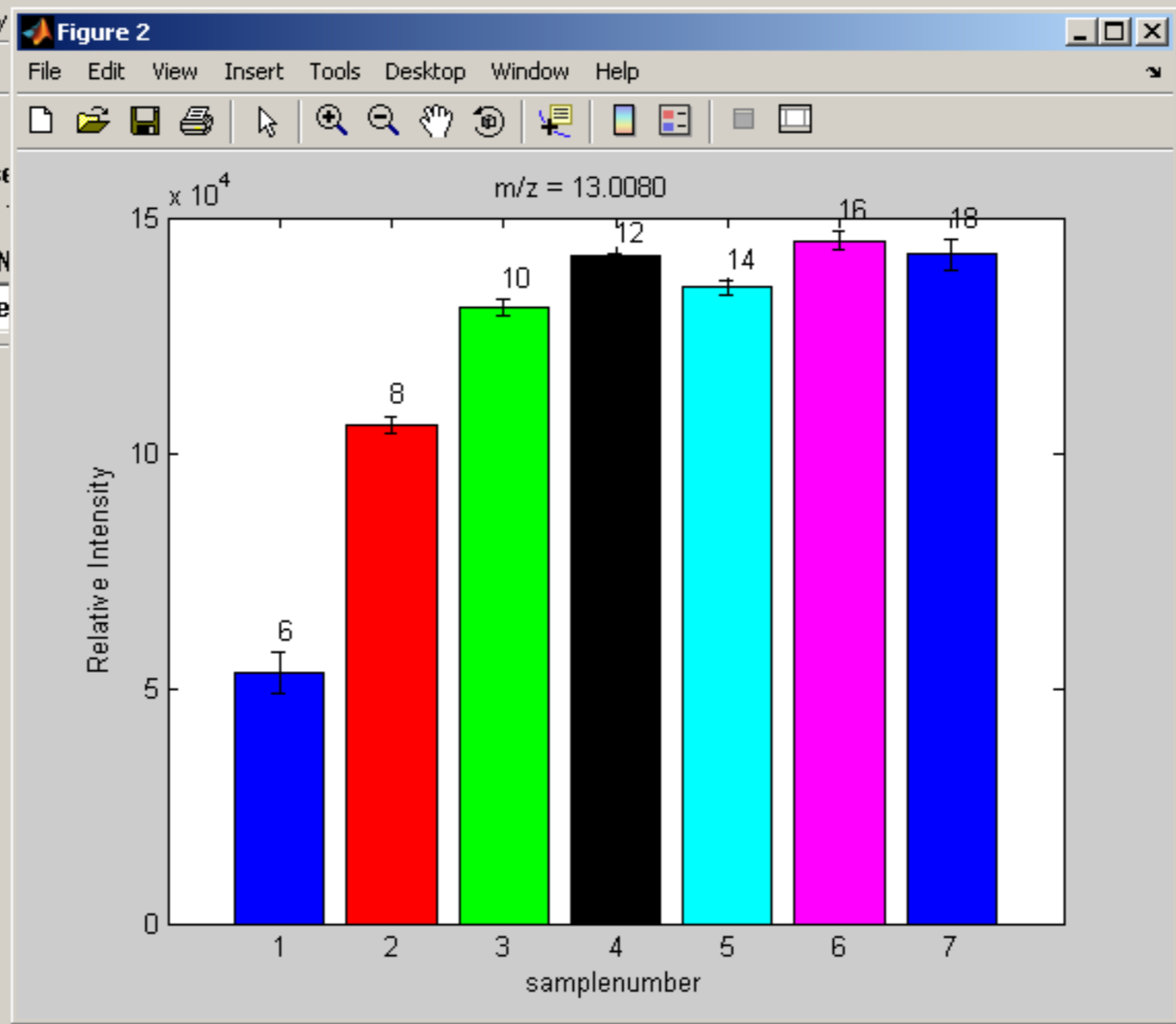
Generate Figure names

25\_0078\_C2H

JPG

Make Figures

Close Panel



Name of Samplenames Matrix

samplenames



Shortcuts How to Add

Workspace



- Name
- data
- exactmass
- filenames
- i
- newdata
- newfiles
- newsamples
- nommass
- peaklabels
- peakstoplot
- samplenames
- totalcounts

Current Directory Workspace

Command History

```

> %-- 10/6/10 3:44
> peakstoplot
> peaklables
> clc
> peakstoplot
> peaklabels
> clc
> peakstoplot
> peaklabels

```

work

File Edit View Favorites Tools Help

Back Forward Stop Refresh Home Print Copy Paste Delete Move

Search Folders

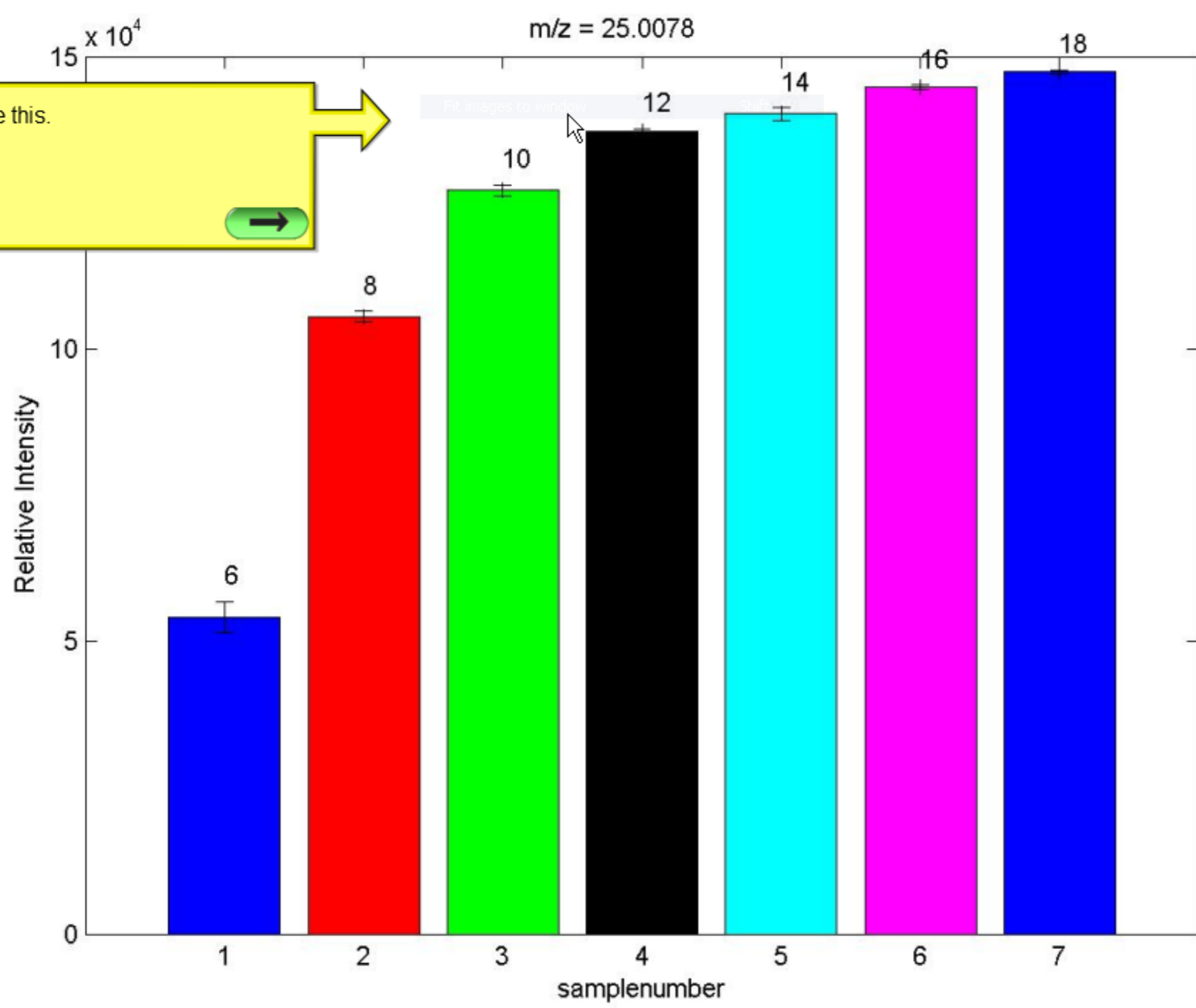
Address C:\Program Files\MATLAB\R2006b\work

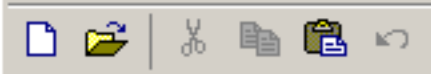
Name	Size	Type	Date Modified
TIMAGE.BIF	8,580 KB	BIF File	4/29/2010 2:15 F
TESTP04.bif	77,961 KB	BIF File	7/16/2010 7:57 /
S1200_03.BIF	10,114 KB	BIF File	9/9/2010 3:53 PF
S1200_01.BIF	10,114 KB	BIF File	9/9/2010 3:47 PF
S103.BIF	3,202 KB	BIF File	3/18/2010 4:57 F
S11P3.BIF	7,428 KB	BIF File	8/17/2010 10:48
S11P2.BIF	7,428 KB	BIF File	8/17/2010 10:47
S11P1.BIF	7,428 KB	BIF File	8/17/2010 10:45
S11N1.BIF	11,557 KB	BIF File	8/18/2010 8:31 /
S10P1.BIF	7,428 KB	BIF File	8/17/2010 10:49
S2GL_09.BIF	21,763 KB	BIF File	9/8/2010 1:40 PF
S2GL_08.BIF	12,290 KB	BIF File	9/9/2010 4:04 PF
S2GL_07.BIF	10,114 KB	BIF File	9/9/2010 3:34 PF
S2GL_06.BIF	5,443 KB	BIF File	9/8/2010 1:38 PF
S2GL_05.BIF	2,946 KB	BIF File	9/8/2010 2:57 PF
S1GL_06.BIF	21,763 KB	BIF File	9/8/2010 1:42 PF
S1GL_05.BIF	10,114 KB	BIF File	9/9/2010 3:43 PF
S1GL_04.BIF	12,290 KB	BIF File	9/9/2010 4:06 PF
S1_02.BIF	7,492 KB	BIF File	3/2/2010 3:31 PF
NA2100_2.BIF	112,012 KB	BIF File	1/4/2010 4:48 PF
MT1_5.BIF	18,050 KB	BIF File	7/8/2010 1:24 PF
J1N.BIF	3,841 KB	BIF File	9/2/2010 10:41 /
F1N.BIF	3,841 KB	BIF File	9/2/2010 10:41 /
	2,817 KB	BIF File	1/4/2010 4:48 PF
	4,097 KB	BIF File	9/2/2010 10:24 /
	4,097 KB	BIF File	9/2/2010 10:24 /
	16,898 KB	BIF File	5/11/2010 9:00 /
	3,841 KB	BIF File	9/2/2010 10:24 /
	3,841 KB	BIF File	9/2/2010 10:40 /
	4,097 KB	BIF File	9/2/2010 10:23 /
	2,945 KB	BIF File	6/28/2010 12:17
1TEST.BIF	18,434 KB	BIF File	3/10/2010 12:18
codeforzoh...sfg.asv	2 KB	ASV File	7/28/2010 2:24 F
25_0078_C2H.jpg	61 KB	JPEG Image	10/7/2010 3:29 F
24_0008_OH.jpg	62 KB	JPEG Image	10/7/2010 3:29 F
17_0030_O.jp	60 KB	JPEG Image	10/7/2010 3:29 F
15_9963_CH3	61 KB	JPEG Image	10/7/2010 3:29 F
14_0162_CH2.jpg	61 KB	JPEG Image	10/7/2010 3:29 F
13_0080_CH.jpg	61 KB	JPEG Image	10/7/2010 3:29 F
11_9999_C.jpg	60 KB	JPEG Image	10/7/2010 3:29 F

All of the figures are in the active Matlab directory and have the names we created previously.

Dimensions: 1200 x 900  
Type: JPEG Image  
Size: 60.0 KB

They look like this.





Shortcuts How to Add

Workspace



Name

- data
- exactmass
- filenames
- i
- newdata
- newfiles
- newsamples
- nommass
- peaklabels
- peakstoplot
- samplenames
- totalcounts

Current Directory

Workspace

Command History

```

-- 10/6/10 3:44
peakstoplot
peaklables
clc
peakstoplot
peaklabels
clc
peakstoplot
peaklabels

```

### 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
data	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.

←      →

