

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

These are the main input data that will be used in further analysis unless you specify otherwise.
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Name of Data Matrix

Name of Variable Matrix

Name of Filename Matrix



Name of Totalcounts Matrix

Name of Samplenames Matrix

This tutorial will show how to use the Ratio Maker Panel of the Spectragui.

This panel allows the user to create ratios of the form $A/(A+B)$ or A/B for any combination of peaks.

This tutorial assumes you have already loaded data and created samplenames.



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

Name of Data Matrix

data

exactmass

specify otherwise.
in your analysis.

counts Matrix

Name of Samplenames Matrix

samplenames

To start, choose:
'Data Display' - > 'Calculate/Plot Peak Ratios'

← →

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="data"/>	<input type="text" value="exactmass"/>	<input type="text" value="filenames"/>	<input type="text" value="totalcounts"/>	<input type="text" value="samplenames"/>

Load Selected Data

Loaded Data:	None
Loaded Samplenames:	None
Loaded Variables:	None

Select Ratio Type

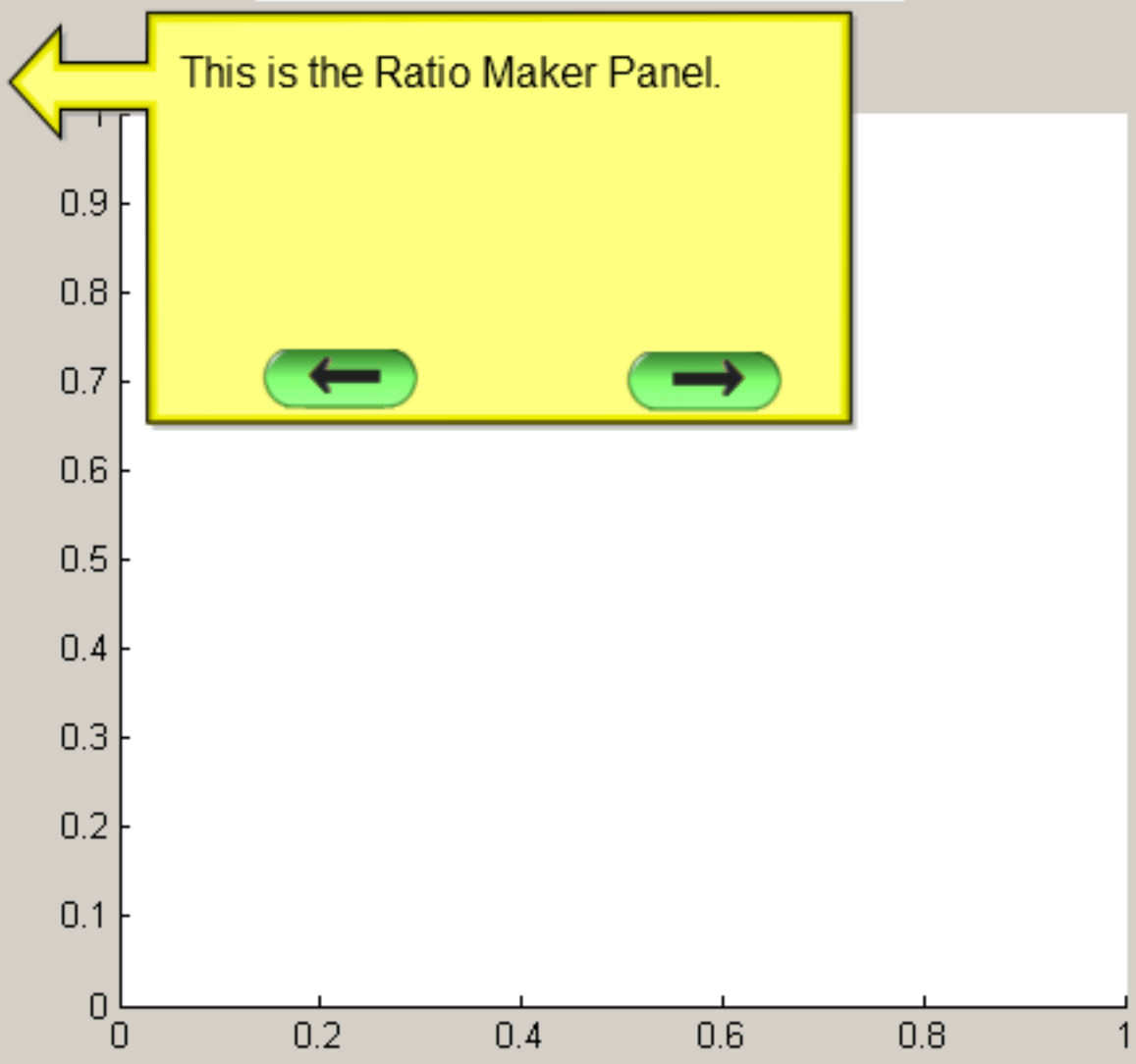
Choose peaks for the ratio.
Multi-select with 'ctrl' or 'shft' key

"A" Peaks

"B" Peaks

Calculate Ratio Export Ratio Data

Select Plot Type



Plot Ratio

EXT Plot

Save Plot to File

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
data	exactmass	filenames	totalcounts	samplenames

Load Selected Data

After selecting the data you want to use from the drop down menus in the Data Selection Panel, press the 'Load Selected Data' button to load the data into the panel.

Loaded Data:	None
Loaded Samplenames:	None
Loaded Variables:	None

Select Plot Type

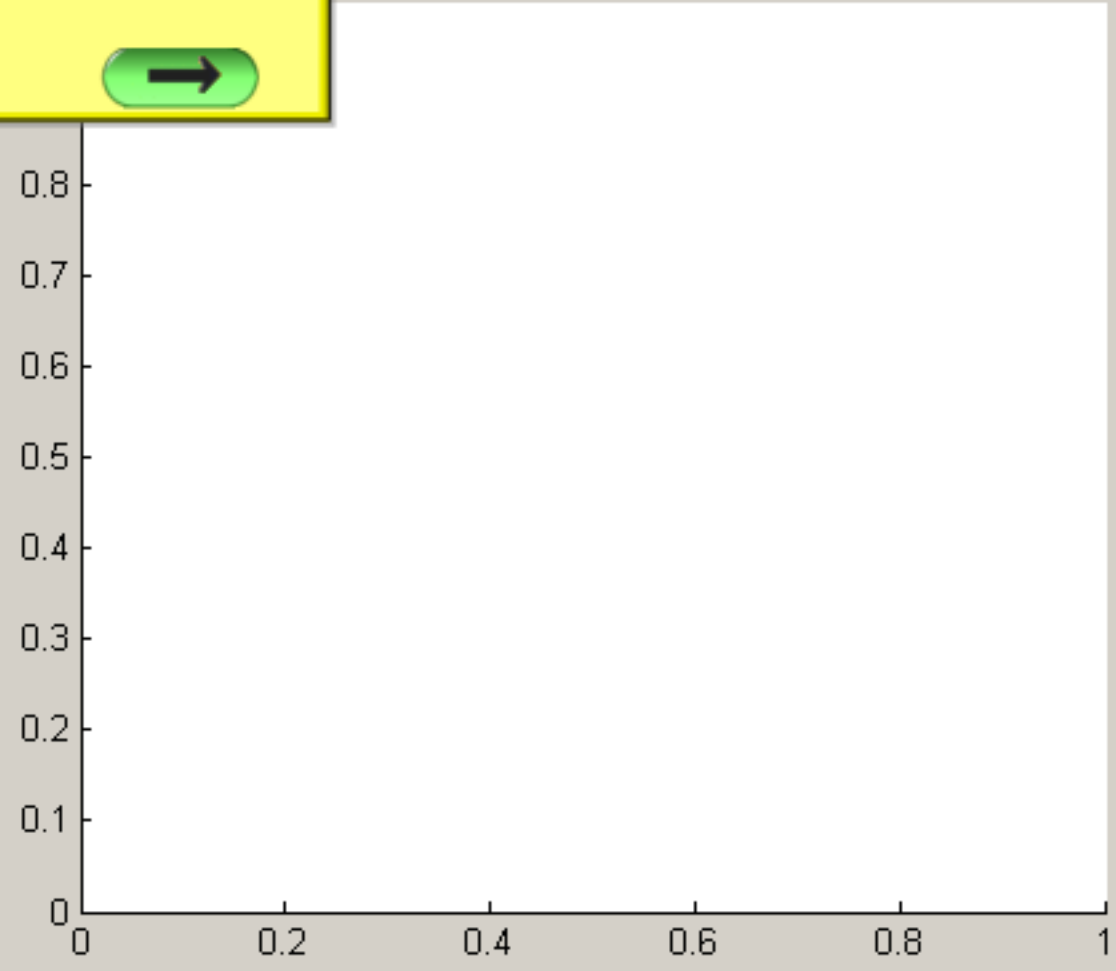
Plot Style

Select Ratio Type

Choose Ratio Type

Choose peaks for the ratio.
Multi-select with 'ctrl' or 'shft' key

"A" Peaks	"B" Peaks
<div style="border: 1px solid gray; height: 100px;"></div>	<div style="border: 1px solid gray; height: 100px;"></div>



Calculate Ratio Export Ratio Data

Plot Ratio EXT Plot

Save Plot to File 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.

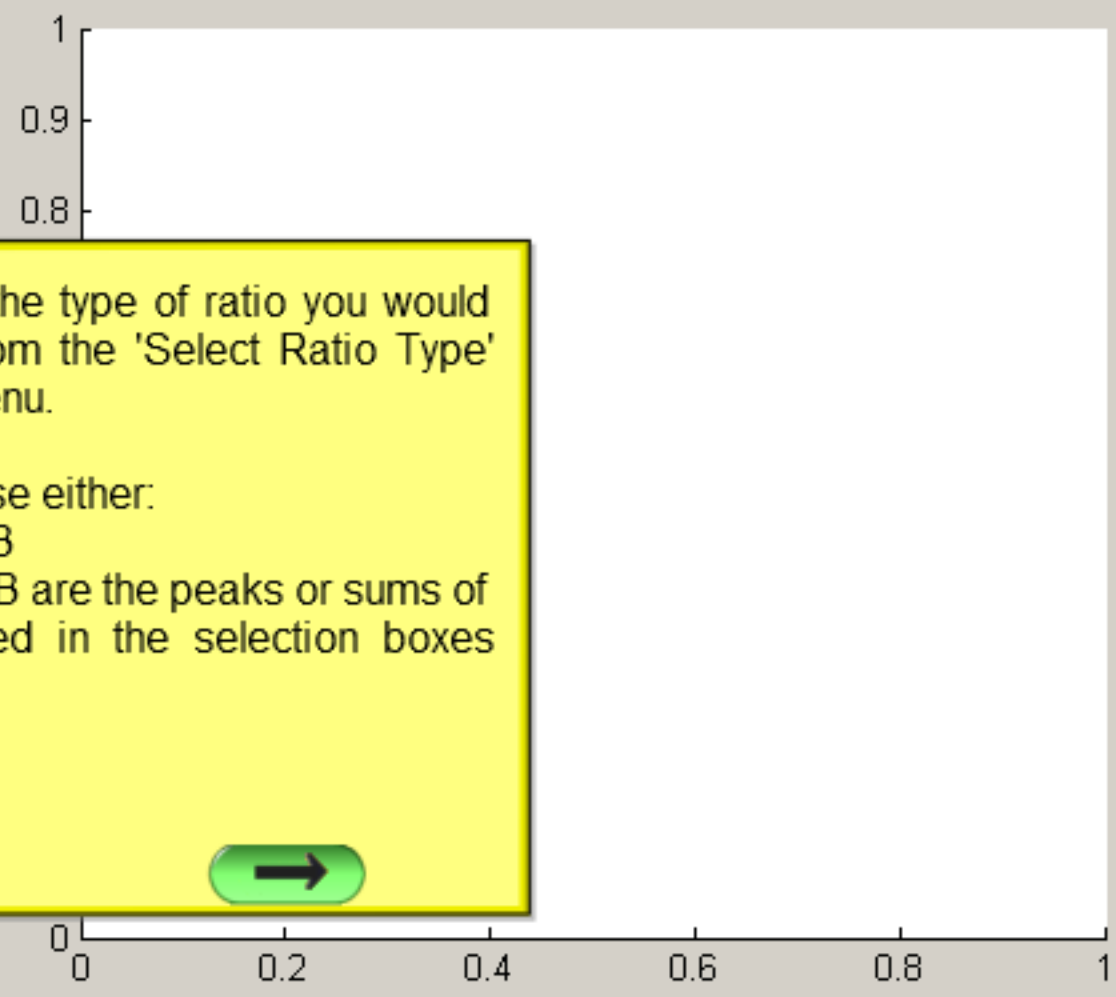
Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

Load Selected Data

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

Select Plot Type

Choose Plot Style



Select Ratio Type

Choose Ratio Type
 Choose Ratio Type
 A / (A + B)
 A / B

Now choose the type of ratio you would like to use from the 'Select Ratio Type' drop down menu.

You can choose either:
 A/(A+B) or A/B
 Where A and B are the peaks or sums of peaks selected in the selection boxes below.

"A" Peaks

"B" Peaks

- 12
- 13
- 14
- 16
- 17
- 24
- 25
- 32
- 33
- 35
- 36
- 37
- 38
- 39
- 46
- 49
- 51
- 57
- 59
- 62
- 80
- 96

- 12
- 13
- 14
- 16
- 17
- 24
- 25
- 32
- 33
- 35
- 36
- 37
- 38
- 39
- 46
- 49
- 51
- 57
- 59
- 62
- 80
- 96

Calculate Ratio Export Ratio Data

Plot Ratio

EXT Plot

Save Plot to File

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.

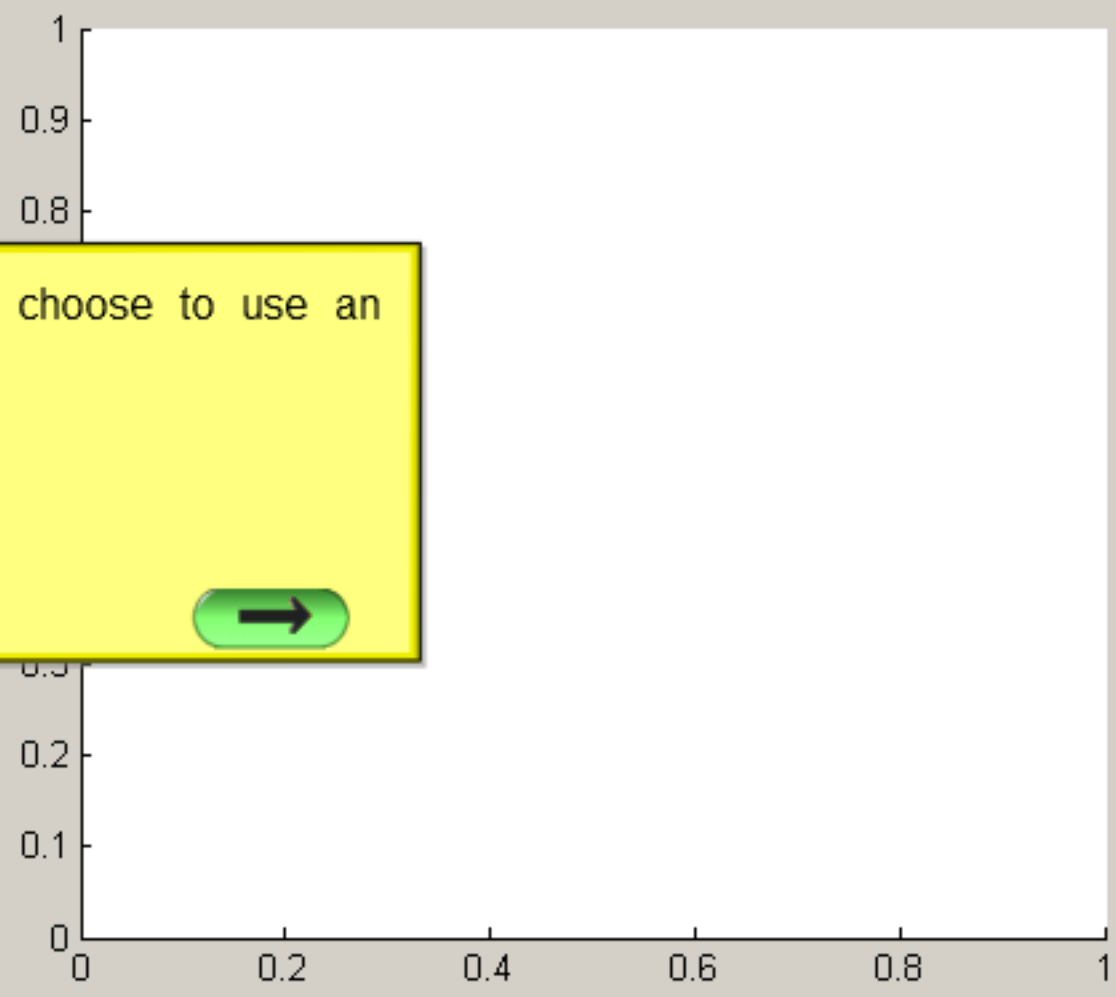
Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

Load Selected Data

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

Select Plot Type

Choose Plot Style



Select Ratio Type

Choose Ratio Type
 Choose Ratio Type
 A / (A + B)
 A / B

Here we will choose to use an A/(A+B) ratio.

"A" Peaks

"B" Peaks

- 12
- 13
- 14
- 16
- 17
- 24
- 25
- 32
- 33
- 35
- 36
- 37
- 38
- 39
- 46
- 49
- 51
- 57
- 59
- 62
- 80
- 96

- 12
- 13
- 14
- 16
- 17
- 24
- 25
- 32
- 33
- 35
- 36
- 37
- 38
- 39
- 46
- 49
- 51
- 57
- 59
- 62
- 80
- 96

Calculate Ratio

Export Ratio Data

Plot Ratio

EXT Plot

Save Plot to File

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
<input type="text" value="data"/>	<input type="text" value="exactmass"/>	<input type="text" value="filenames"/>	<input type="text" value="totalcounts"/>	<input type="text" value="samplenames"/>

Load Selected Data

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

Select Ratio Type

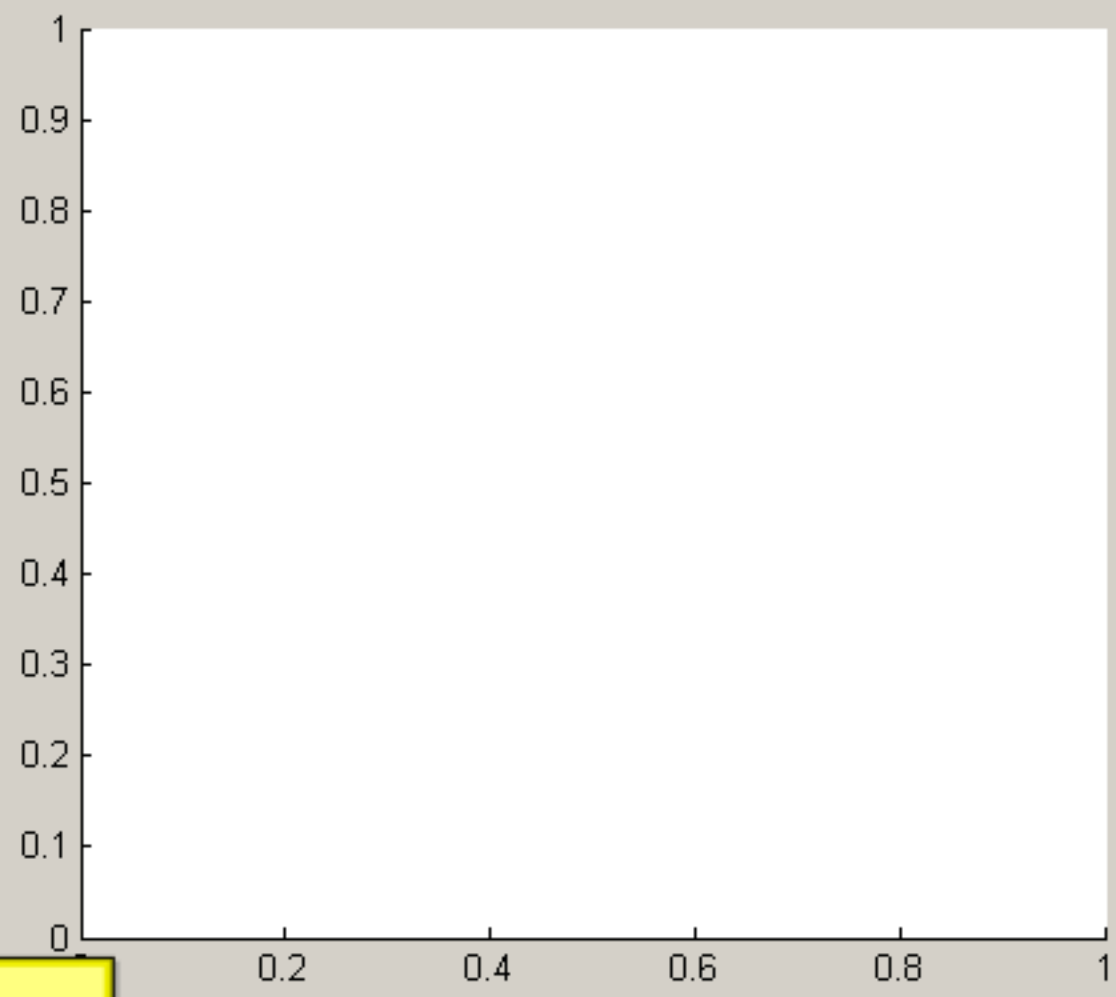
Choose peaks for the ratio.
Multi-select with 'ctrl' or 'shft' key

- "A" Peaks
- 394
 - 399
 - 426
 - 427
 - 431
 - 455
 - 458
 - 483
 - 487
 - 490
 - 511
 - 539
 - 543
 - 567
 - 591
 - 595
 - 599
 - 623
 - 623
 - 651
 - 655
 - 655

- "B" Peaks
- 12
 - 13
 - 14
 - 16
 - 17
 - 24
 - 25
 - 32
 - 33
 - 35
 - 36
 - 37
 - 48
 - 49
 - 51
 - 53
 - 59
 - 62
 - 80
 - 98

Next select the peaks you want to use for "A" peaks in the ratio.
You can select multiple peaks by using the 'ctrl' or 'shift' keys.

Select Plot Type



Plot Ratio

EXT Plot

Save Plot to File

Close Panel

Calculate Ratio

Export Ratio Data

Data Selection Panel

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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:

Load Selected Data

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

Select Ratio Type

Choose peaks for the ratio.
Multi-select with 'ctrl' or 'shft' key

"A" Peaks:

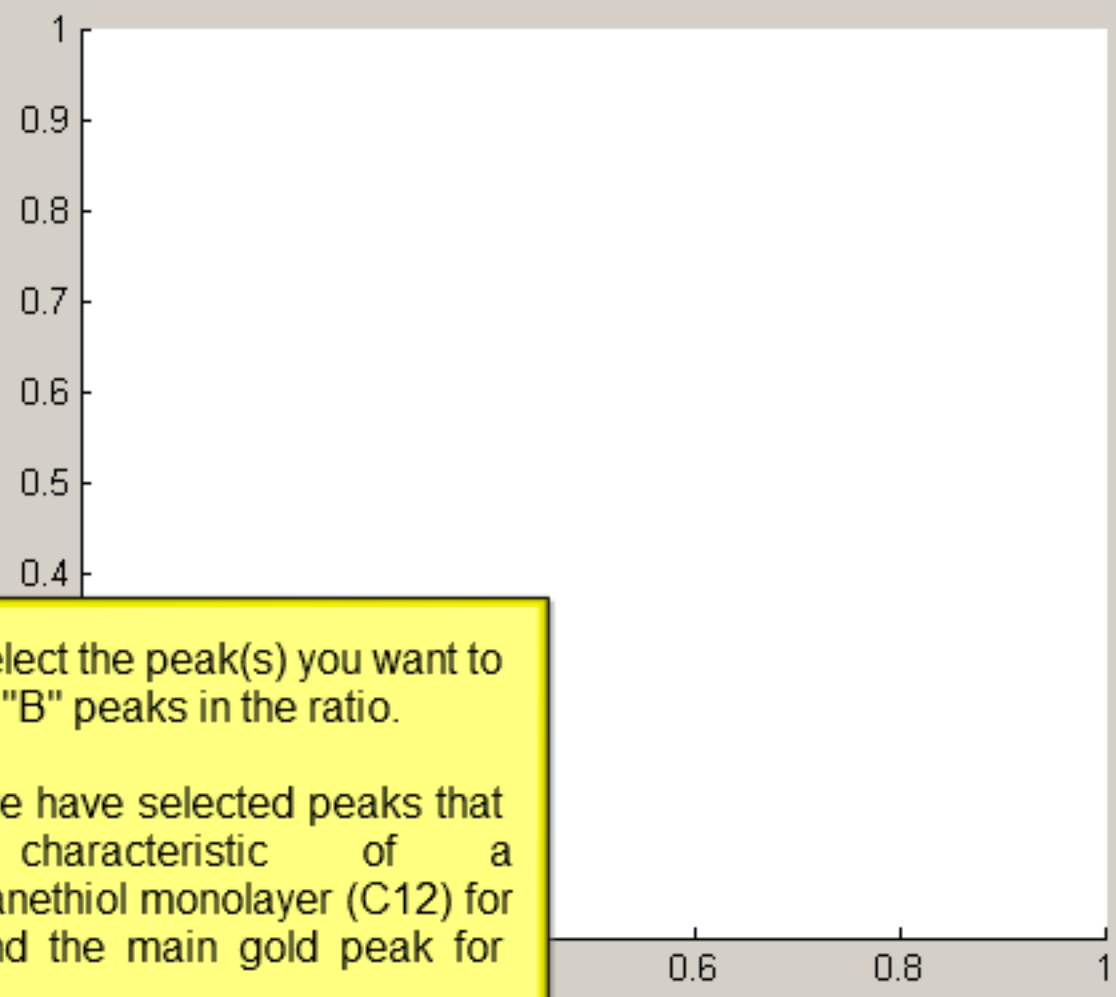
"B" Peaks:

Next select the peak(s) you want to use for "B" peaks in the ratio.

Here we have selected peaks that are characteristic of a dodecanethiol monolayer (C12) for "A", and the main gold peak for "B".



Select Plot Type



Calculate Ratio Export Ratio Data

Save Plot to File EXT Plot Close Panel

Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
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Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

Load Selected Data

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

Select Plot Type

Choose Plot Style

Select Ratio Type

A / (A + B)

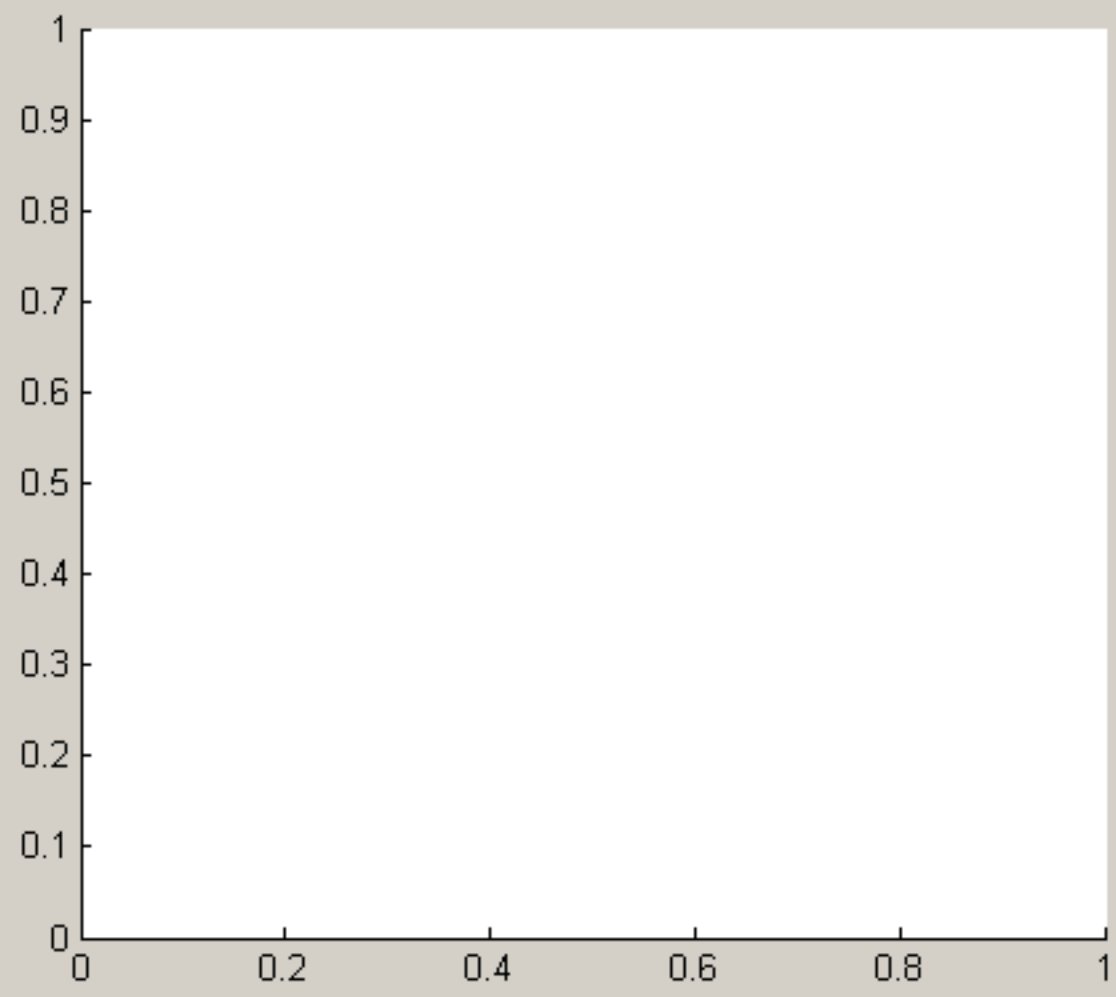
Choose peaks for the ratio.
Multi-select with 'ctrl' or 'shft' key

"A" Peaks

- 394
- 399
- 426
- 427
- 431
- 455
- 458
- 483
- 487
- 490
- 511
- 539
- 543
- 567
- 591
- 595
- 599
- 623
- 623
- 651
- 655
- 655

"B" Peaks

- 193
- 197
- 201
- 221
- 229
- 229
- 249
- 257
- 261
- 277
- 285
- 293
- 305
- 315
- 333
- 343
- 358
- 371
- 394
- 399
- 426
- 427



Calculate Ratio

Export

Plot Ratio

EXT Plot

Save Plot to File

Close Panel

After selecting the desired peaks, press the 'Calculate Ratio' button.



Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise.
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Name of Data Matrix: Name of Variable Matrix: Name of Filename Matrix: Name of Totalcounts Matrix: Name of Samplenames Matrix:

Load Selected Data

Select Plot Type

Loaded Data:
Loaded Samplenames: **sa**
Loaded Variables: **ex**

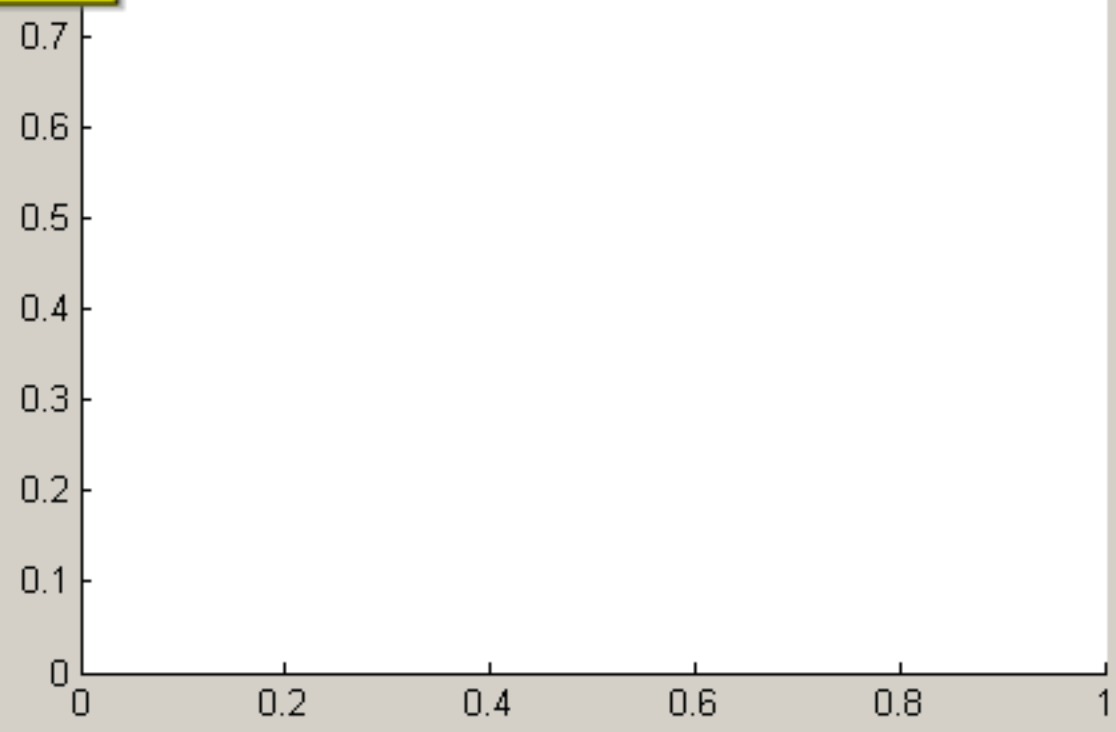
In order to view the data, first select the type of plot you want from the 'Select Plot Type' drop down menu.

Choose Plot Style
Choose Plot Style
Scatter
Bar
Average + Stdev
Average + Stdev Colored

Select Ratio Type: ← →

Choose peaks for the ratio.
Multi-select with 'ctrl' or 'shft' key

"A" Peaks	"B" Peaks
394	193
399	197
426	201
427	221
431	229
455	229
458	249
483	257
487	261
490	277
511	285
539	293
543	305
567	315
591	333
595	343
599	358
623	371
623	394
651	399
655	426
655	427



Calculate Ratio Export Ratio Data

Plot Ratio EXT Plot
Save Plot to File 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:

Load Selected Data

Loaded Data: **data**
Loaded Samplenames: **samplenames**
Loaded Variables:

Select Ratio

Choose peaks for the ratio.
Multi-select with 'ctrl' or 'shft' key

- "A" Peaks
- 394
 - 399
 - 426
 - 427
 - 431
 - 455
 - 458
 - 483
 - 487
 - 490
 - 511
 - 539
 - 543
 - 567
 - 591
 - 595
 - 599
 - 623
 - 623
 - 651
 - 655
 - 655

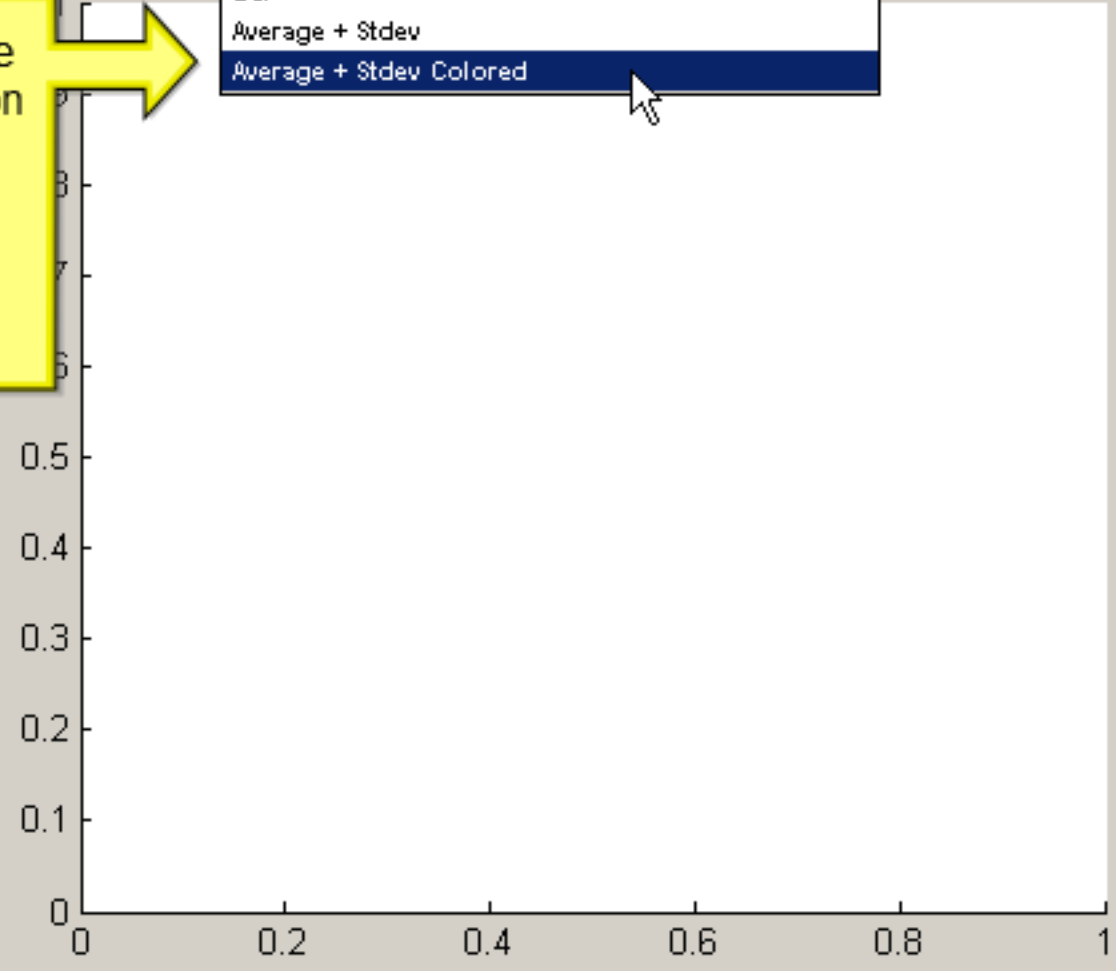
- "B" Peaks
- 193
 - 197
 - 201
 - 221
 - 229
 - 229
 - 249
 - 257
 - 261
 - 277
 - 285
 - 293
 - 305
 - 315
 - 333
 - 343
 - 358
 - 371
 - 394
 - 399
 - 426
 - 427

Calculate Ratio Export Ratio Data

Select Plot Type

Choose Plot Style
Choose Plot Style
Scatter
Bar
Average + Stdev
Average + Stdev Colored

Here we select to show the average and standard deviation using colored bars.



Plot Ratio

EXT Plot

Save Plot to File

Close Panel

Data Selection Panel

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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="data"/>	<input type="text" value="exactmass"/>	<input type="text" value="filenames"/>	<input type="text" value="totalcounts"/>	<input type="text" value="samplenames"/>

Load Selected Data

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

Select Plot Type

Select Ratio Type

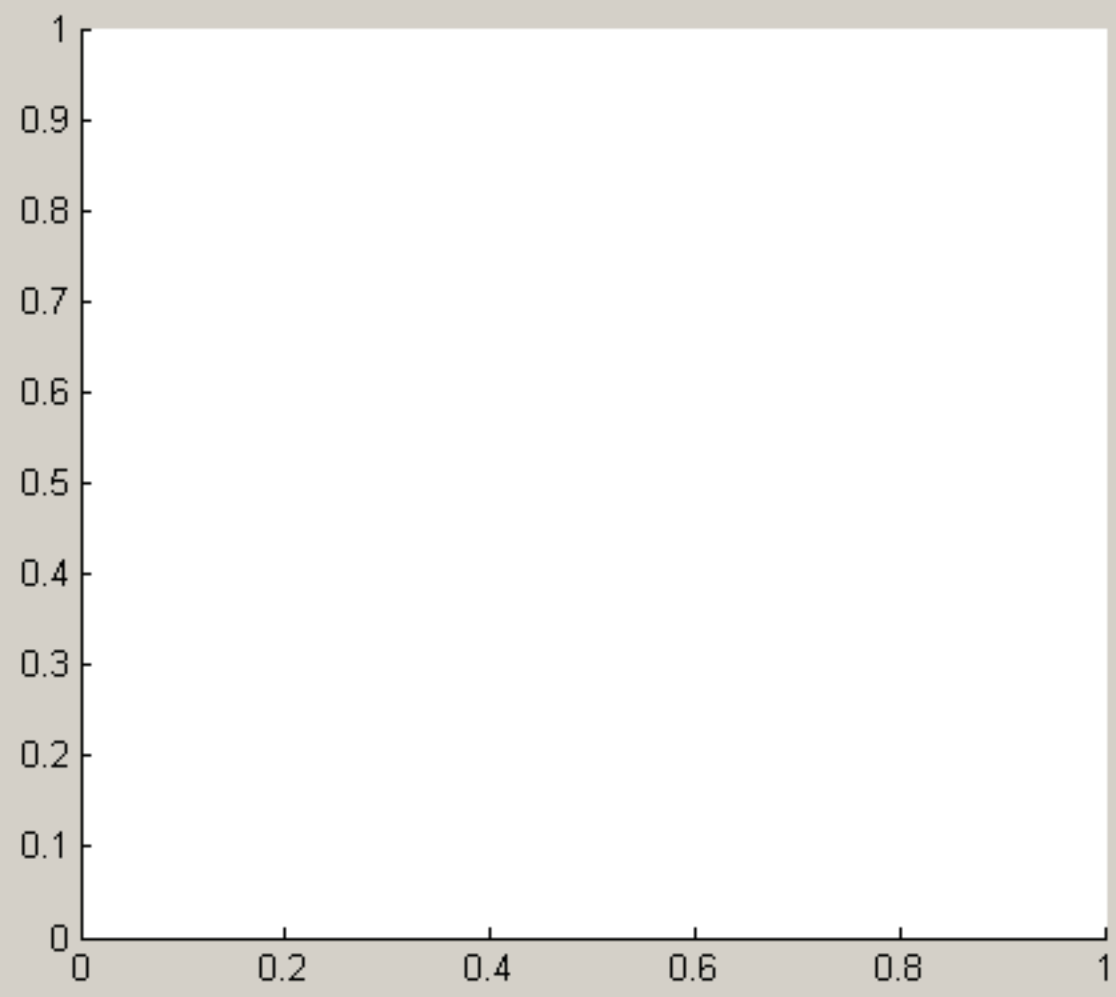
Choose peaks for the ratio.
Multi-select with 'ctrl' or 'shft' key

"A" Peaks

- 394
- 399
- 426
- 427
- 431
- 455
- 458
- 483
- 487
- 490
- 511
- 539
- 543
- 567
- 591
- 595
- 599
- 623
- 623
- 651
- 655
- 655

"B" Peaks

- 193
- 197
- 201
- 221
- 229
- 229
- 249
- 257
- 261
- 277
- 285
- 293
- 305
- 315
- 333



Press the 'Plot Ratio' button to view the data.

Calculate Ratio



Plot Ratio

EXT Plot

Save Plot to File

Close Panel

Data Selection Panel

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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:

Load Selected Data

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

Select Ratio Type

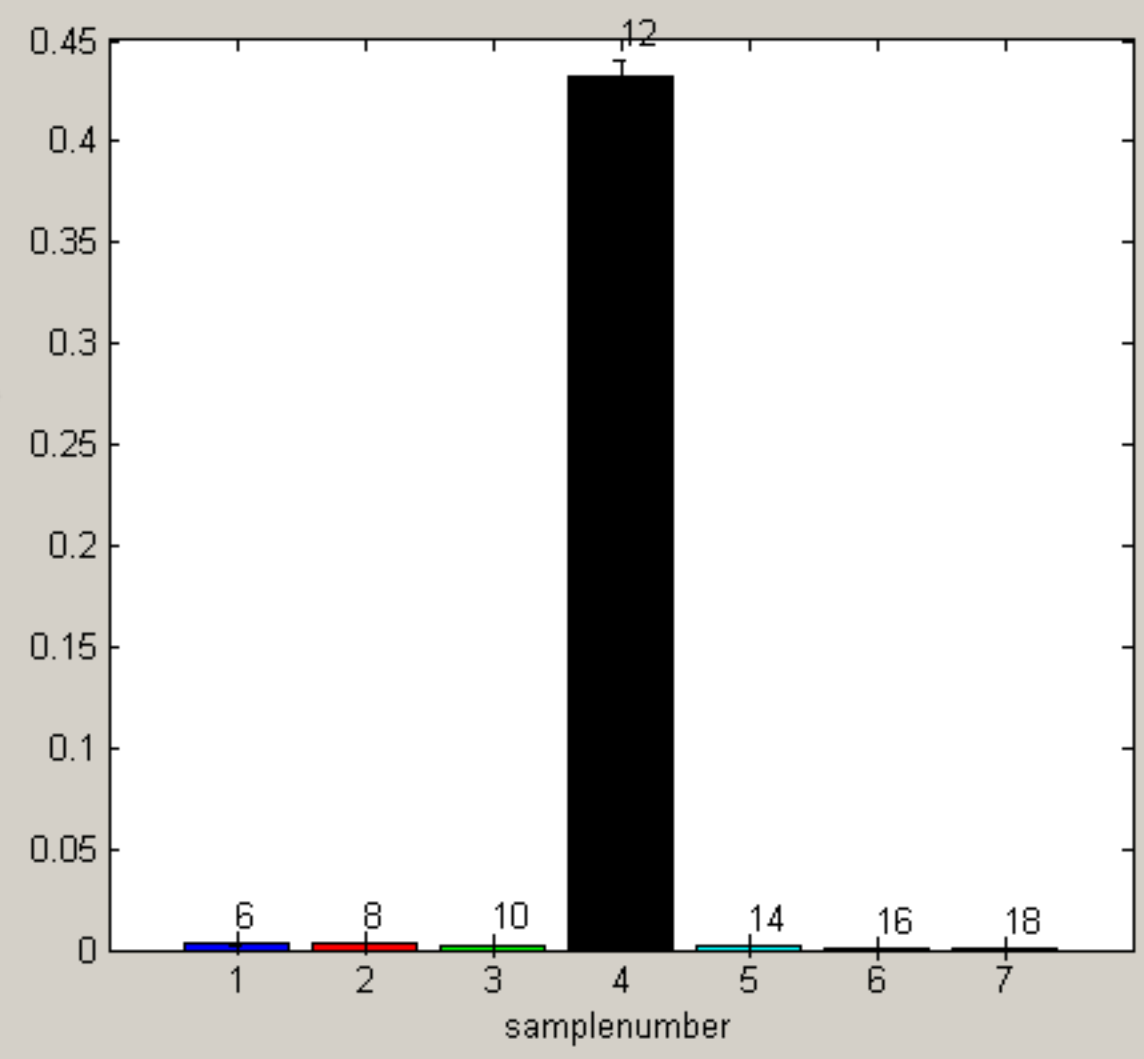
The data is displayed here.

Ch
Multi
"A" Pe

394	229
399	229
426	249
427	257
431	261
455	277
458	285
483	293
487	305
490	315
511	333
539	343
543	358
567	371
591	394
595	399
599	426
623	427
623	
651	
655	
655	

Calculate Ratio Export Ratio Data

Select Plot Type



Plot Ratio

EXT Plot

Save Plot to File

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
<input type="text" value="data"/>	<input type="text" value="exactmass"/>	<input type="text" value="filenames"/>	<input type="text" value="totalcounts"/>	<input type="text" value="samplenames"/>

Load Selected Data

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

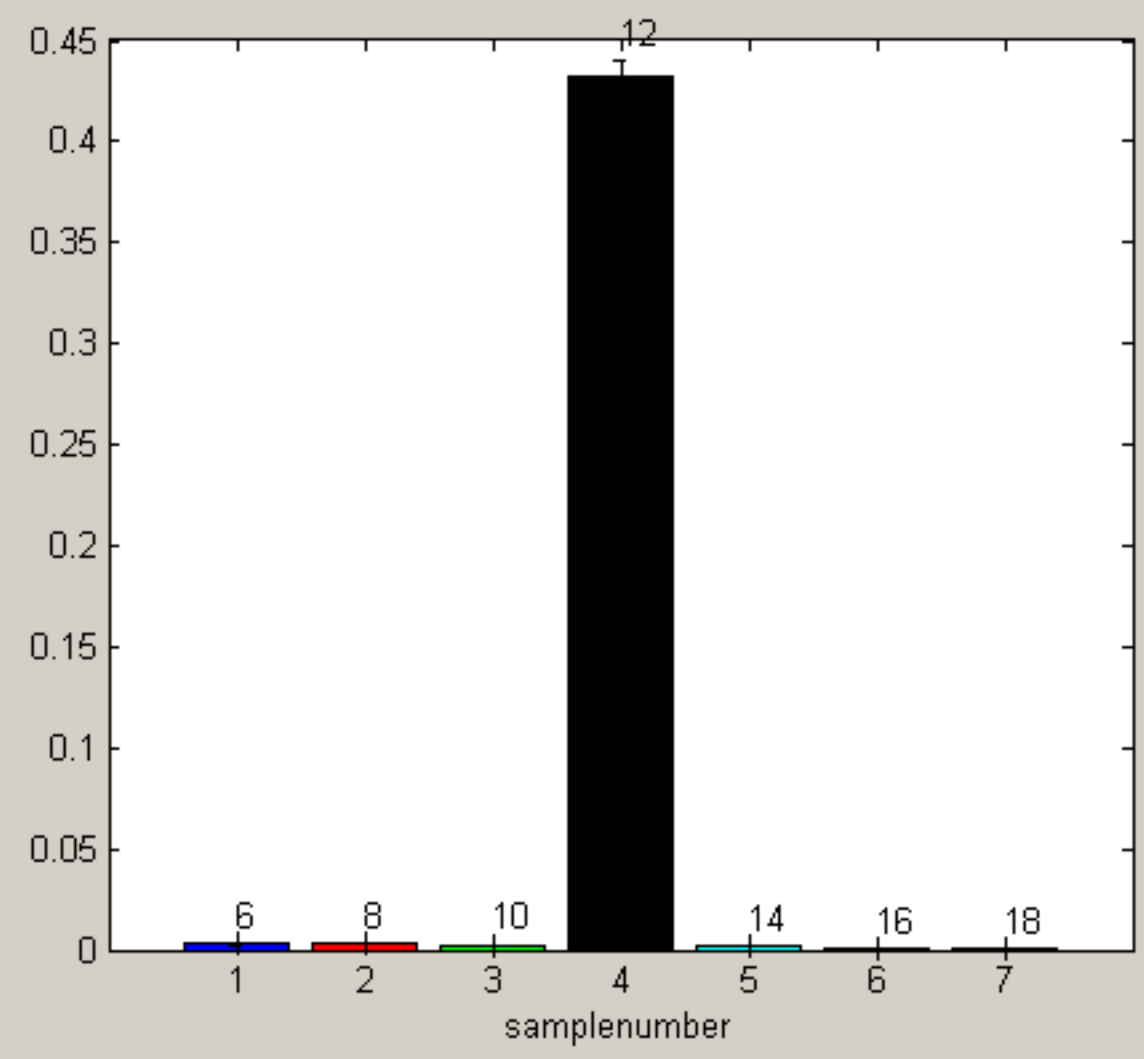
Select Ratio Type

Choose peaks for the ratio.
Multi-select with 'ctrl' or 'shft' key

"A" Peaks	"B" Peaks
<input type="text" value="394"/> <input type="text" value="399"/> <input type="text" value="426"/> <input type="text" value="427"/> <input type="text" value="431"/> <input type="text" value="455"/> <input type="text" value="458"/> <input type="text" value="483"/> <input type="text" value="487"/> <input type="text" value="490"/> <input type="text" value="511"/> <input type="text" value="539"/> <input type="text" value="543"/> <input type="text" value="567"/> <input type="text" value="591"/> <input type="text" value="595"/> <input type="text" value="599"/> <input type="text" value="623"/> <input type="text" value="623"/> <input type="text" value="651"/> <input type="text" value="655"/> <input type="text" value="655"/>	<input type="text" value="193"/> <input type="text" value="197"/> <input type="text" value="201"/> <input type="text" value="221"/> <input type="text" value="229"/> <input type="text" value="229"/> <input type="text" value="249"/> <input type="text" value="257"/> <input type="text" value="261"/> <input type="text" value="277"/> <input type="text" value="285"/> <input type="text" value="293"/> <input type="text" value="305"/> <input type="text" value="315"/> <input type="text" value="333"/> <input type="text" value="343"/> <input type="text" value="358"/> <input type="text" value="371"/> <input type="text" value="394"/> <input type="text" value="399"/> <input type="text" value="426"/> <input type="text" value="427"/>

Calculate Ratio Export Ratio Data

Select Plot Type



You can create a plot in a separate window using the 'Ext Plot' button.

EXT Plot
Close Panel



spectragui
File Data Pre-Processing MVA Data Display

Data :
These are the main input data that will
Use the drop down menus to select the

Name of Data Matrix: Name of Variable Matrix: Name:

Load Selected Data

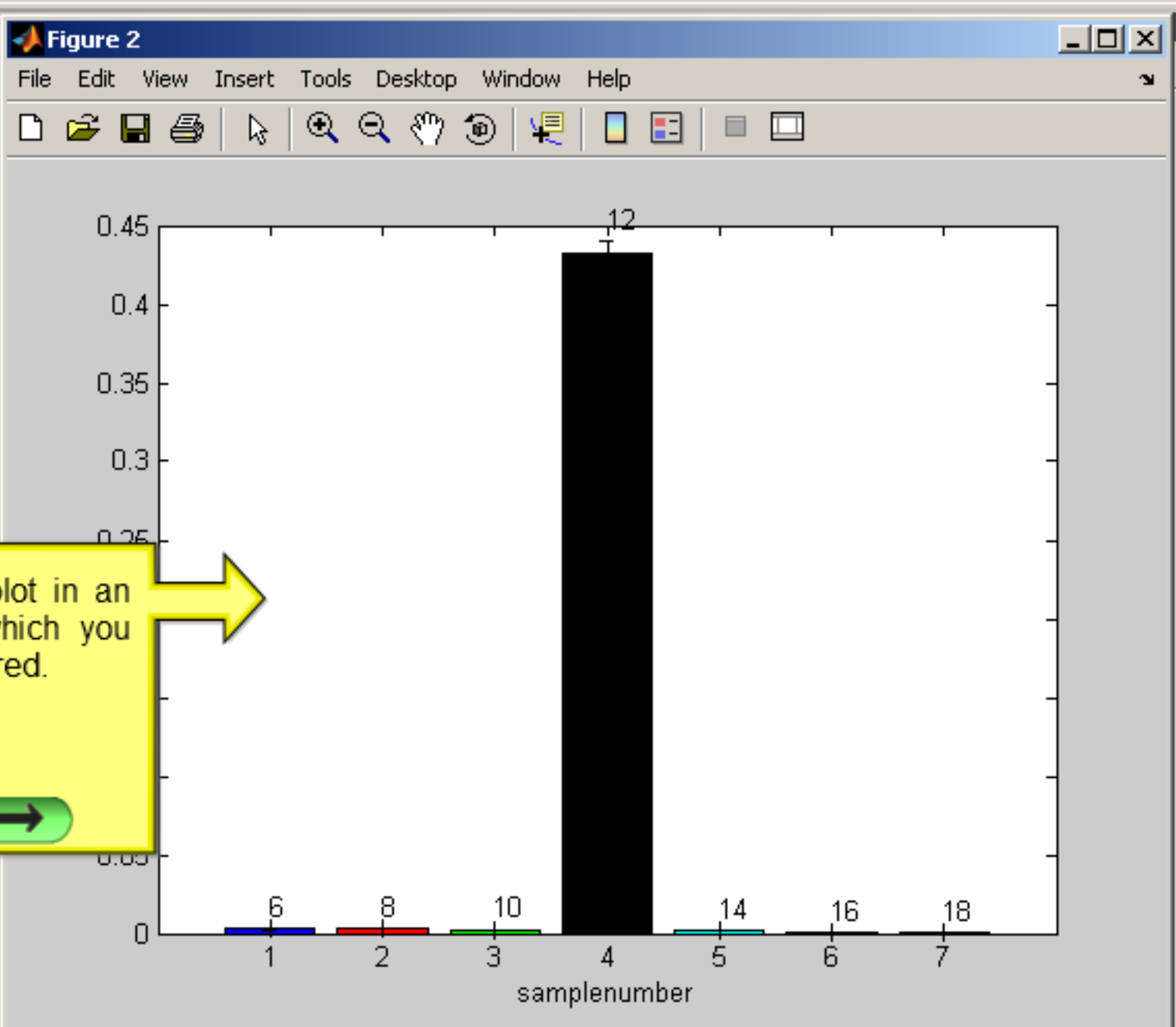
Loaded Data:
Loaded Samplenames: sar
Loaded Variables: ex

Select Ratio Type: ← →

Choose peaks for the ratio.
Multi-select with 'ctrl' or 'shft' key

"A" Peaks	"B" Peaks
394	193
399	197
426	201
427	221
431	229
455	229
458	249
483	257
487	261
490	277
511	285
539	293
543	305
567	315
591	333
595	343
599	358
623	371
623	394
651	399
655	426
655	427

Calculate Ratio **Export Ratio Data**



Samplenumber	Ratio
1	0.01
2	0.01
3	0.01
4	0.18
5	0.01
6	0.01
7	0.01

Plot Ratio **EXT Plot**
Save Plot to File **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:

Load Selected Data

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

Select Ratio Type

Choose peaks for the ratio.
Multi-select with 'ctrl' or 'shft' key

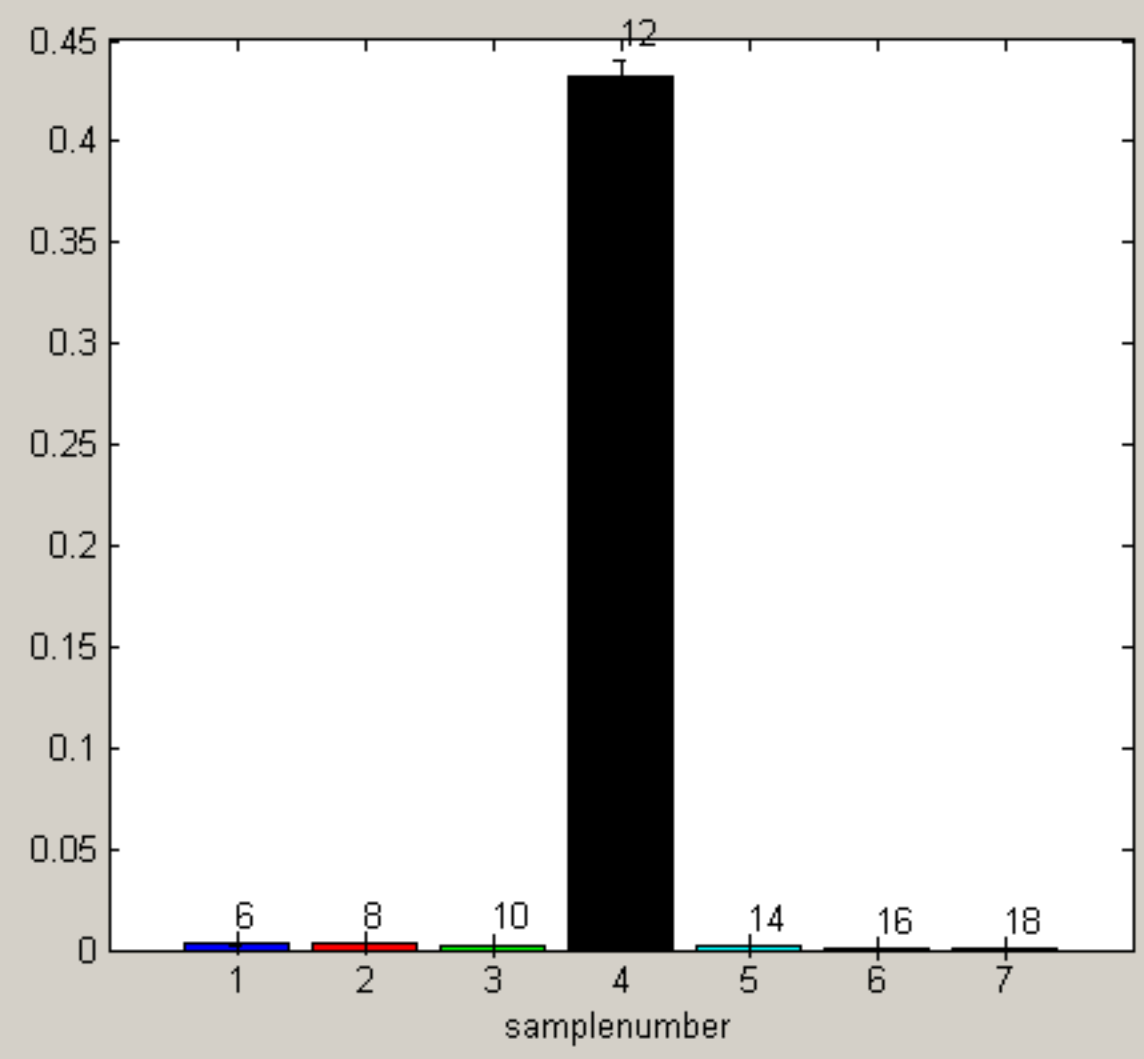
- "A" Peaks
- 394
 - 399
 - 426
 - 427
 - 431
 - 455
 - 458
 - 483
 - 487
 - 490
 - 511
 - 539
 - 543
 - 567
 - 591
 - 595
 - 599
 - 623
 - 623
 - 651
 - 655
 - 655

- "B" Peaks
- 193
 - 197
 - 201
 - 221
 - 229
 - 229
 - 249
 - 257
 - 261
 - 277
 - 285
 - 293
 - 305
 - 315
 - 333
 - 343
 - 358
 - 371
 - 394
 - 399
 - 411
 - 411

Calculate Ratio

Ex

Select Plot Type



Plot Ratio

EXT Plot

Save Plot to File

Close Panel

You can also save the figure using the 'Save Plot to File' button.



Save picture as

Save in: work

- frames
- OverlayXYSnapshot.jpg

File name: C12toAuratio

Save as type: jpeg (*.jpg)

Save Cancel

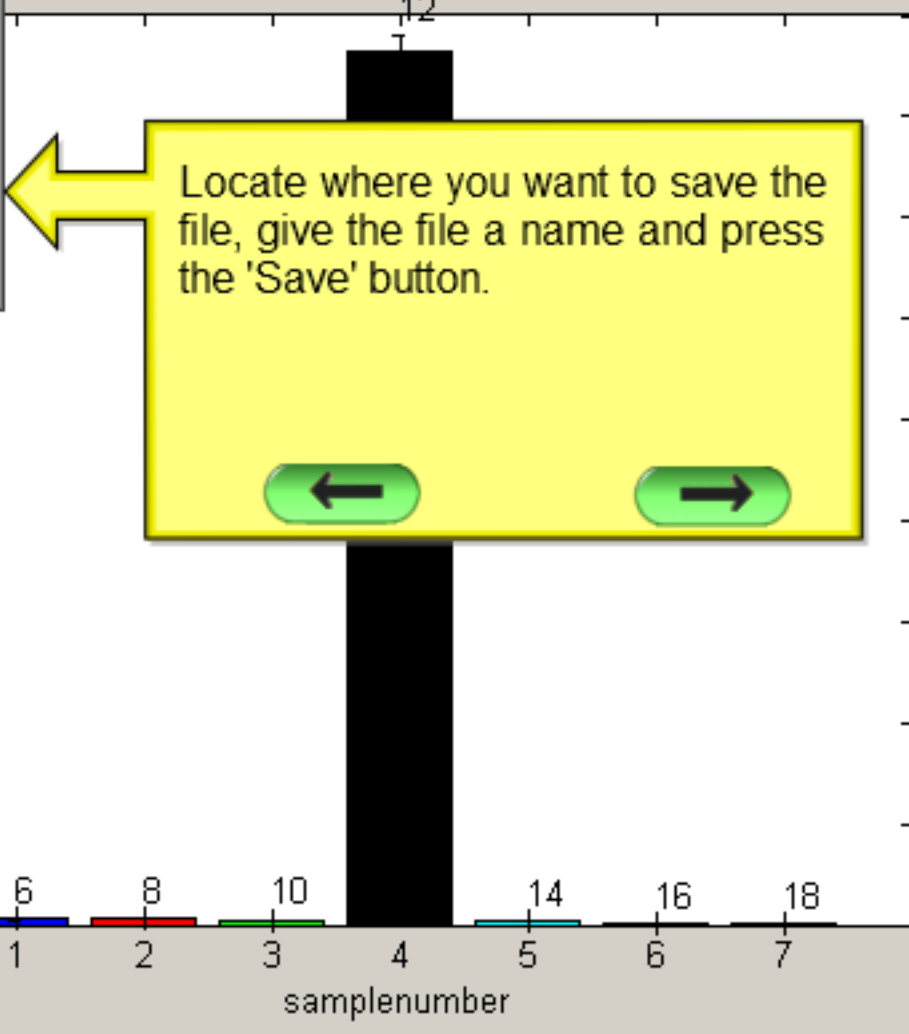
Panel

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

Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
	totalcounts	samplenames

Select Plot Type

Average + Stdev Colored



Locate where you want to save the file, give the file a name and press the 'Save' button.

Choose peaks for the ratio.

Multi-select with 'ctrl' or 'shft' key

"A" Peaks	"B" Peaks
394	193
399	197
426	201
427	221
431	229
455	229
458	249
483	257
487	261
490	277
511	285
539	293
543	305
567	315
591	333
595	343
599	358
623	371
623	394
651	399
655	426
655	427

Calculate Ratio Export Ratio Data

Plot Ratio EXT Plot

Save Plot to File Close Panel

work

File Edit View Favorites Tools Help

Back Search Folders

Address C:\Program Files

C12toAuratio.jpg - IrfanView (Zoom: 595 x 446)

File Edit Image Options View Help

sample number	Value
1	0.01
2	0.02
3	0.03
4	0.43
5	0.01
6	0.01
7	0.01

No file loaded (use File->Open menu)

File Name	Size	Type	Date Modified
test3.txt	7 KB	Text Do...	1/3/2011 5:25 PM
testv6.txt	15 KB	Text Do...	10/11/2010 2:15 P
v6fortutorial.txt	15 KB	Text Do...	10/11/2010 3:39 P
ysampledata.txt	1 KB	Text Do...	10/13/2010 11:57
Corr3dviewSnapShot.tif	747 KB	TIF File	6/24/2011 12:06 P
3drotationmovie.avi	380,75...	Video Clip	6/24/2011 3:56 PM
RGBOverlayMovie.avi	380,75...	Video Clip	6/23/2011 10:36 A
XYRGBOverlaymovie.avi	39,280 KB	Video Clip	6/23/2011 10:34 A
C12toAuratio.jpg	40 KB	JPG File	7/13/2011 12:47 P

The file is saved with the given name in the chosen directory.

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="data"/>	<input type="text" value="exactmass"/>	<input type="text" value="filenames"/>	<input type="text" value="totalcounts"/>	<input type="text" value="samplenames"/>

Load Selected Data

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

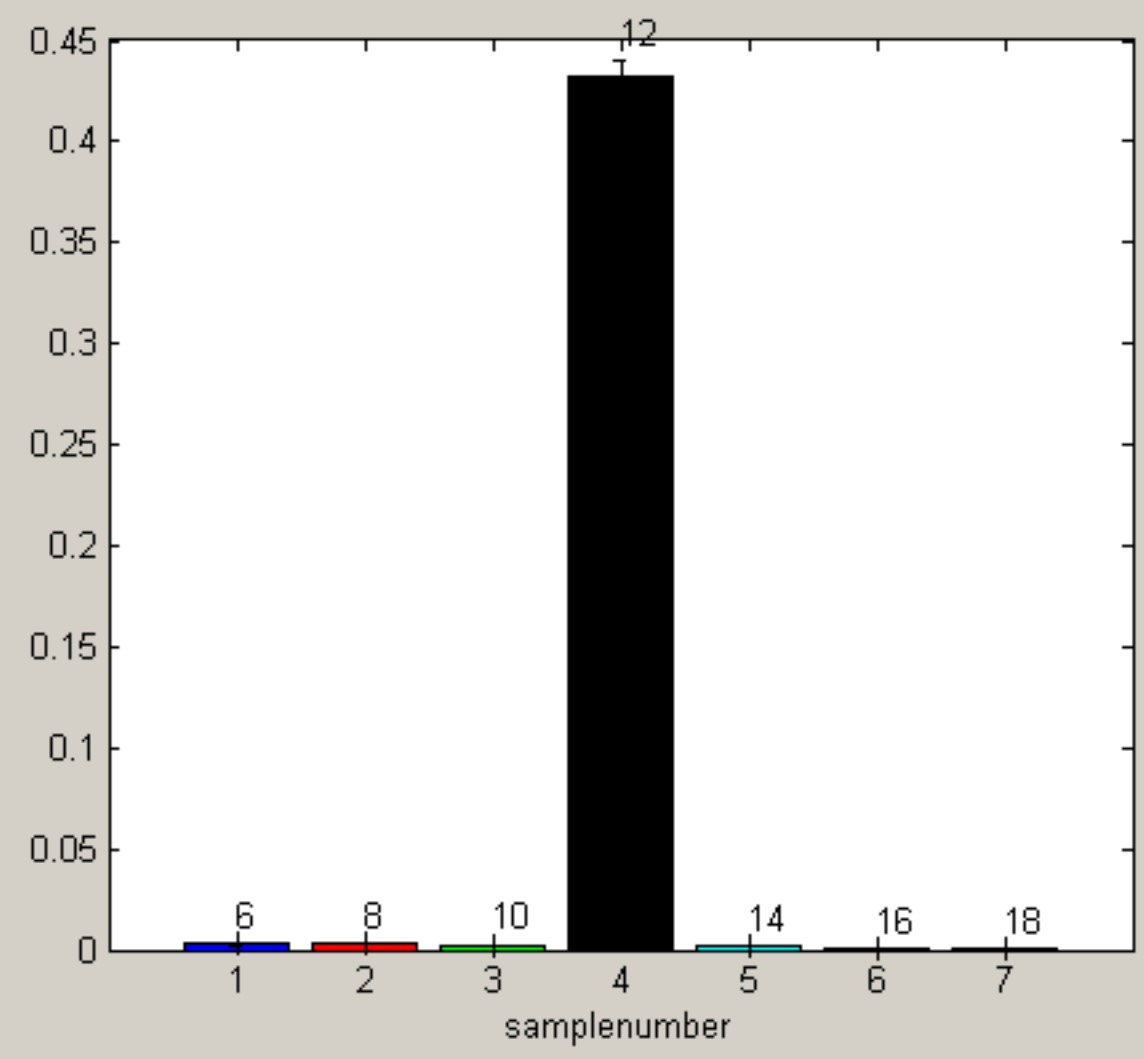
Select Ratio Type

Choose peaks for the ratio.
Multi-select with 'ctrl' or 'shft' key

"A" Peaks	"B" Peaks
<input type="text" value="394"/> <input type="text" value="399"/> <input type="text" value="426"/> <input type="text" value="427"/> <input type="text" value="431"/> <input type="text" value="455"/> <input type="text" value="458"/> <input type="text" value="483"/> <input type="text" value="487"/> <input type="text" value="490"/> <input type="text" value="511"/> <input type="text" value="539"/> <input type="text" value="543"/> <input type="text" value="567"/> <input type="text" value="591"/> <input type="text" value="595"/> <input type="text" value="599"/> <input type="text" value="623"/> <input type="text" value="623"/> <input type="text" value="651"/> <input type="text" value="655"/> <input type="text" value="655"/>	<input type="text" value="193"/> <input type="text" value="197"/> <input type="text" value="201"/> <input type="text" value="221"/> <input type="text" value="229"/> <input type="text" value="229"/> <input type="text" value="249"/> <input type="text" value="257"/> <input type="text" value="261"/> <input type="text" value="277"/> <input type="text" value="285"/> <input type="text" value="293"/> <input type="text" value="305"/> <input type="text" value="315"/> <input type="text" value="333"/> <input type="text" value="343"/> <input type="text" value="358"/> <input type="text" value="371"/> <input type="text" value="394"/> <input type="text" value="399"/> <input type="text" value="426"/> <input type="text" value="427"/>

Calculate Ratio **Export Ratio Data**

Select Plot Type



Plot Ratio EXT Plot

Close Panel

You can export the ratio data to an ascii text file by pressing the 'Export Ratio Data' button.



Save file as

Save in: work

- frames
- AcuNegData.txt
- AcuPosData.txt
- AllNeg20110131.txt
- allpeaksimpos.txt
- AllPos20110131.txt
- asbposdata.txt
- BAS_C60_neg_6.txt
- BAS_C60_pos_6.txt
- BASControlNEG17.txt
- BASControlPos20.txt
- bv.txt
- CH3NEV.TXT
- controldata.txt
- fortutorial.txt
- FRE-HYD-old.TXT
- Gel_NegData_25.txt
- Gel_PosData_26.txt
- iontof.txt
- it6files.txt
- la.txt
- negative.txt
- NegativeInkdata_95.txt
- negnewdata.txt
- NEGTEST.TXT
- newcln.txt
- newlabelsmethane.txt
- NHS-BARE.TXT
- positive.txt
- pp1314neg.txt
- pp1314pos.txt
- prueba99.txt
- redpos.txt
- sa.txt
- test3.txt
- testv6.txt
- v6fortutorial.txt
- ysampledata.txt

File name: C12toAuratio

Save as type: txt (*.txt)

Save Cancel

Panel

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

Matrix	Name of Totalcounts Matrix	Name of Samplenames Matrix
	totalcounts	samplenames

Select Plot Type

Average + Stdev Colored

Sample Number	Peak Height
1	0.01
2	0.01
3	0.01
4	0.30
5	0.01
6	0.01
7	0.01

Choose where to save the file, give the file a name and press the 'Save' button.

Choose peaks for the ratio.

Multi-select with 'ctrl' or 'shft' key

"A" Peaks	"B" Peaks
394	193
399	197
426	201
427	221
431	229
455	229
458	249
483	257
487	261
490	277
511	285
539	293
543	305
567	315
591	333
595	343
599	358
623	371
623	394
651	399
655	426
655	427

Calculate Ratio Export Ratio Data

Sample Number	Peak Height
1	0.01
2	0.01
3	0.01
4	0.30
5	0.01
6	0.01
7	0.01

Plot Ratio EXT Plot

Save Plot to File Close Panel

C12toAuratio.txt - WordPad

File Edit View Insert Format Help



0.00259
0.00267
0.00387
0.00259
0.00267
0.00387
0.00310
0.00325
0.00308
0.00310
0.00325
0.00308
0.00258
0.00251
0.00261
0.00258
0.00251
0.00261
0.42597
0.44177
0.42832
0.42597
0.44177
0.42832
0.00166
0.00156
0.00166
0.00166
0.00156
0.00166
0.00084
0.00110
0.00085
0.00084
0.00110
0.00085
0.00088
0.00100
0.00089
0.00088
0.00100
0.00089
A / (A + B)
A P e a k s
595
599
B P e a k s
197

The data is saved along with a description of what data was used in the ratio.

File Edit View Insert Format Help



Go

name	Size	Type	Date Modified
BAS_C60_neg_6.txt	7 KB	Text Do...	6/29/2011 2:20 PM
BAS_C60_pos_6.txt	14 KB	Text Do...	6/29/2011 2:15 PM
BASControlNEG17.txt	17 KB	Text Do...	6/28/2011 11:55 A
BASControlPos20.txt	39 KB	Text Do...	6/27/2011 4:59 PM
bv.txt	1 KB	Text Do...	10/13/2010 11:56
CH3NEV.TXT	313 KB	Text Do...	1/4/2010 4:48 PM
controldata.txt	13 KB	Text Do...	4/29/2010 2:21 PM
fortutorial.txt	18 KB	Text Do...	10/11/2010 1:10 P
FRE-HYD-old.TXT	14 KB	Text Do...	8/31/2007 10:49 A
Gel_NegData_25.txt	27 KB	Text Do...	7/7/2011 1:53 PM
Gel_PosData_26.txt	28 KB	Text Do...	7/6/2011 5:08 PM
d2624.log	16 KB	Text Do...	7/8/2010 2:21 PM
d2792.log	16 KB	Text Do...	11/2/2010 4:29 PM
	11 KB	Text Do...	1/27/2010 1:10 PM
	3 KB	Text Do...	8/13/2010 12:56 P
	8 KB	Text Do...	10/13/2010 11:56
	10 KB	Text Do...	8/23/2010 10:24 A
inkdata_95.txt	324 KB	Text Do...	5/4/2011 10:10 AM
ata.txt	34 KB	Text Do...	7/27/2010 11:44 A
.TXT	17 KB	Text Do...	10/11/2010 4:40 P
newcln.txt	54 KB	Text Do...	1/4/2010 4:45 PM
newlabelsmethane.txt	2 KB	Text Do...	2/28/2011 5:10 PM
NHS-BARE.TXT	7 KB	Text Do...	11/8/2007 11:45 A
positive.txt	28 KB	Text Do...	5/8/2011 5:11 PM
pp1314neg.txt	10 KB	Text Do...	3/23/2011 10:55 A
pp1314pos.txt	15 KB	Text Do...	3/23/2011 10:54 A
prueba99.txt	1 KB	Text Do...	12/20/2010 11:11
redpos.txt	17 KB	Text Do...	7/23/2010 5:02 PM
sa.txt	4 KB	Text Do...	10/13/2010 11:56
test3.txt	7 KB	Text Do...	1/3/2011 5:25 PM
testv6.txt	15 KB	Text Do...	10/11/2010 2:15 P
v6fortutorial.txt	15 KB	Text Do...	10/11/2010 3:39 P
ysampledata.txt	1 KB	Text Do...	10/13/2010 11:57
Corr3dviewSnapShot.tif	747 KB	TIF File	6/24/2011 12:06 P
3drotationmovie.avi	380,75...	Video Clip	6/24/2011 3:56 PM
RGBOverlayMovie.avi	380,75...	Video Clip	6/23/2011 10:36 A
XYRGBOverlaymovie.avi	39,280 KB	Video Clip	6/23/2011 10:34 A
C12toAuratio.jpg	40 KB	JPG File	7/13/2011 12:47 P
C12toAuratio.txt	1 KB	Text Do...	7/13/2011 12:48 P

C12toAuratio.txt - WordPad

File Edit View Insert Format Help



0.00259
 0.00267
 0.00387
 0.00259
 0.00267
 0.00387
 0.00310
 0.00325
 0.00308
 0.00310
 0.00325
 0.00308
 0.00258
 0.00251
 0.00261
 0.00258
 0.00251
 0.00261
 0.42597
 0.44177
 0.42832
 0.42597
 0.44177
 0.42832
 0.00166
 0.00156
 0.00166
 0.00166
 0.00156
 0.00166
 0.00166
 0.00156
 0.00166
 0.00084
 0.00110
 0.00085
 0.00084
 0.00110
 0.00085
 0.00088
 0.00100
 0.00089
 0.00088
 0.00100
 0.00089
 A / (A + B)
 A P e a k s
 595
 599
 B P e a k s
 197

File Edit View Insert Format Help



Go

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Gel_NegData_25.txt	27 KB	Text Do...	7/7/2011 1:53 PM
Gel_PosData_26.txt	28 KB	Text Do...	7/6/2011 5:08 PM
hs_err_pid2624.log	16 KB	Text Do...	7/8/2010 2:21 PM
hs_err_pid2792.log	16 KB	Text Do...	11/2/2010 4:29 PM
iontof.txt	11 KB	Text Do...	1/27/2010 1:10 PM
it6files.txt	3 KB	Text Do...	8/13/2010 12:56 P
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NEGTEST.TXT	17 KB	Text Do...	10/11/2010 4:40 P
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positive.txt	28 KB	Text Do...	5/8/2011 5:11 PM
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test3.txt	7 KB	Text Do...	1/3/2011 5:25 PM
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Corr3dviewSnapShot.tif	747 KB	TIF File	6/24/2011 12:06 P
380,75...		Video Clip	6/24/2011 3:56 PM
380,75...		Video Clip	6/23/2011 10:36 A
39,280 KB		Video Clip	6/23/2011 10:34 A
40 KB		JPG File	7/13/2011 12:47 P
1 KB		Text Do...	7/13/2011 12:48 P

The file footer shows the type of ratio used and which peaks were chosen for "A" and "B".



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="data"/>	<input type="text" value="exactmass"/>	<input type="text" value="filenames"/>	<input type="text" value="totalcounts"/>	<input type="text" value="samplenames"/>

Load Selected Data

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

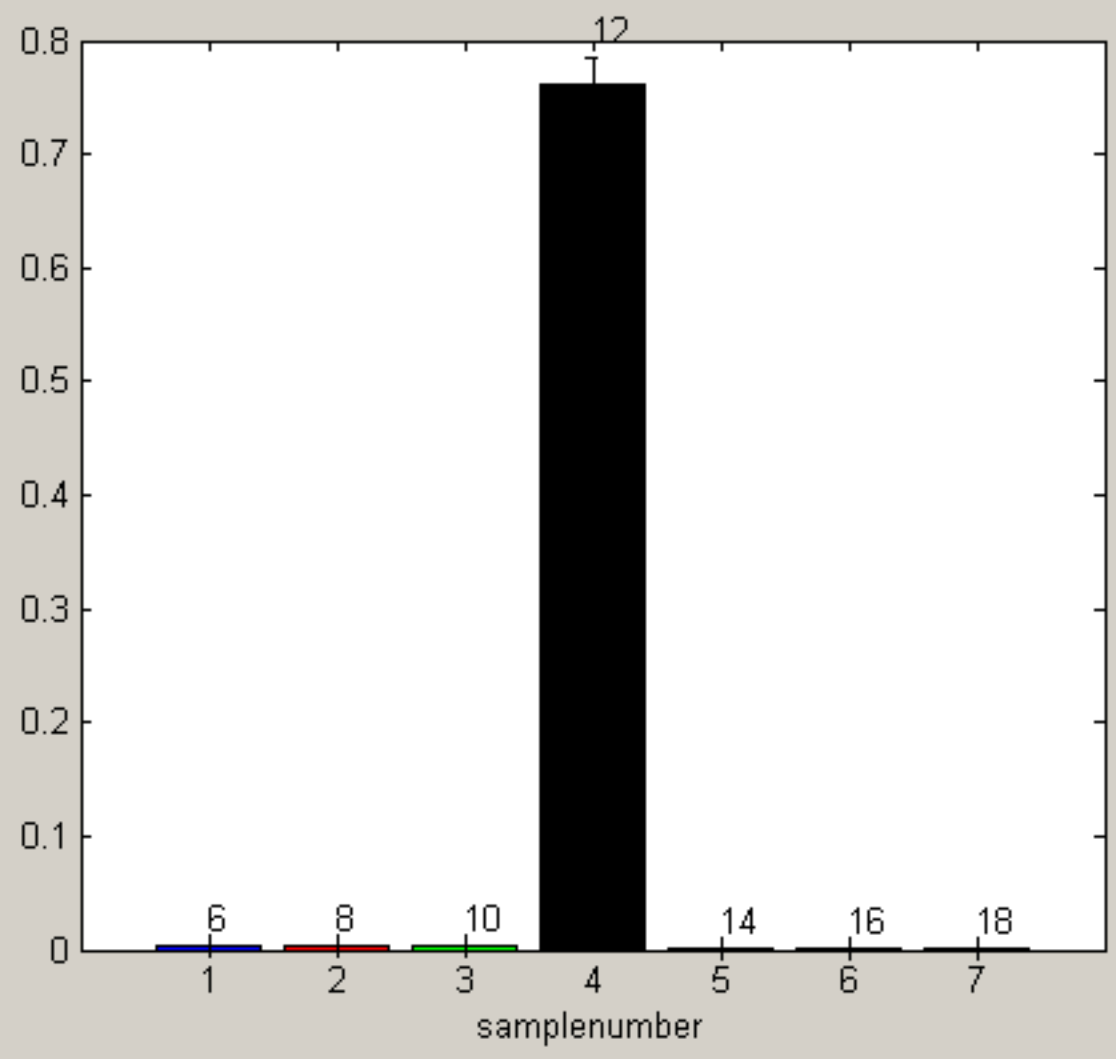
Select Ratio Type

Choose peaks for the ratio.
Multi-select with 'ctrl' or 'shft' key

"A" Peaks	"B" Peaks
<input type="text" value="394"/> <input type="text" value="399"/> <input type="text" value="426"/> <input type="text" value="427"/> <input type="text" value="431"/> <input type="text" value="455"/> <input type="text" value="458"/> <input type="text" value="483"/> <input type="text" value="487"/> <input type="text" value="490"/> <input type="text" value="511"/> <input type="text" value="539"/> <input type="text" value="543"/> <input type="text" value="567"/> <input type="text" value="591"/> <input type="text" value="595"/> <input type="text" value="599"/> <input type="text" value="623"/> <input type="text" value="623"/> <input type="text" value="651"/> <input type="text" value="655"/> <input type="text" value="655"/>	<input type="text" value="193"/> <input type="text" value="197"/> <input type="text" value="201"/> <input type="text" value="221"/> <input type="text" value="229"/> <input type="text" value="229"/> <input type="text" value="249"/> <input type="text" value="257"/> <input type="text" value="261"/> <input type="text" value="277"/> <input type="text" value="285"/> <input type="text" value="293"/> <input type="text" value="305"/> <input type="text" value="315"/> <input type="text" value="333"/> <input type="text" value="343"/> <input type="text" value="358"/> <input type="text" value="371"/> <input type="text" value="394"/> <input type="text" value="399"/> <input type="text" value="426"/> <input type="text" value="427"/>

Calculate Ratio Export Ratio Data

Select Plot Type



Plot Ratio EXT Plot

Close Panel

Press the 'Close' button to close the 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

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.

