

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="ndatat"/>	<input type="text" value="exactmass"/>	<input type="text" value="filenames"/>	<input type="text" value="Select Totalcounts..."/>	<input type="text" value="samplegroups ..."/>

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.
Use the drop down menus to select the data and information you want to use in your analysis.

Name of Data Matrix

ndatat

Name of Variable Matrix

exactmass

Name of Filename Matrix

filenames

Name of Totalcounts Matrix

Select Totalcounts...

Name of Samplenames Matrix

samplegroups ...

This tutorial will cover how to use a function called the correlated peak finder.

The correlated peak finder looks at the average intensity of each peak across all samples and finds all the peaks that show a similar pattern in the relative intensity within a given tolerance.

This function looks at the pattern in the relative intensities and not the absolute relative intensities. It is looking for patterns within the data.

I find this useful to use together with PCA to help find peaks that show the same patterns within a data set.



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

Data Selection Panel

The main input is the name of the matrix you want to use in your analysis.

Name of Data Matrix

ndatat

Name of Variable

exactmass

Name of Totalcounts Matrix

Select Totalcounts...

Name of Samplenames Matrix

samplegroups ...

To start the function choose 'Find Correlated Peaks' from the 'MVA' menu.



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="ndatat"/>	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="Select Totalcounts..."/>	Name of Samplenames Matrix <input type="text" value="samplegroups ..."/>
--	---	---	--	---

Load Selected Data

Current Selection

Data:
Variables:
Samplenames:

Make sure the correct data is selected from the menus above.

← →

Labels to use:

Tolerance value for match (0 to 1)

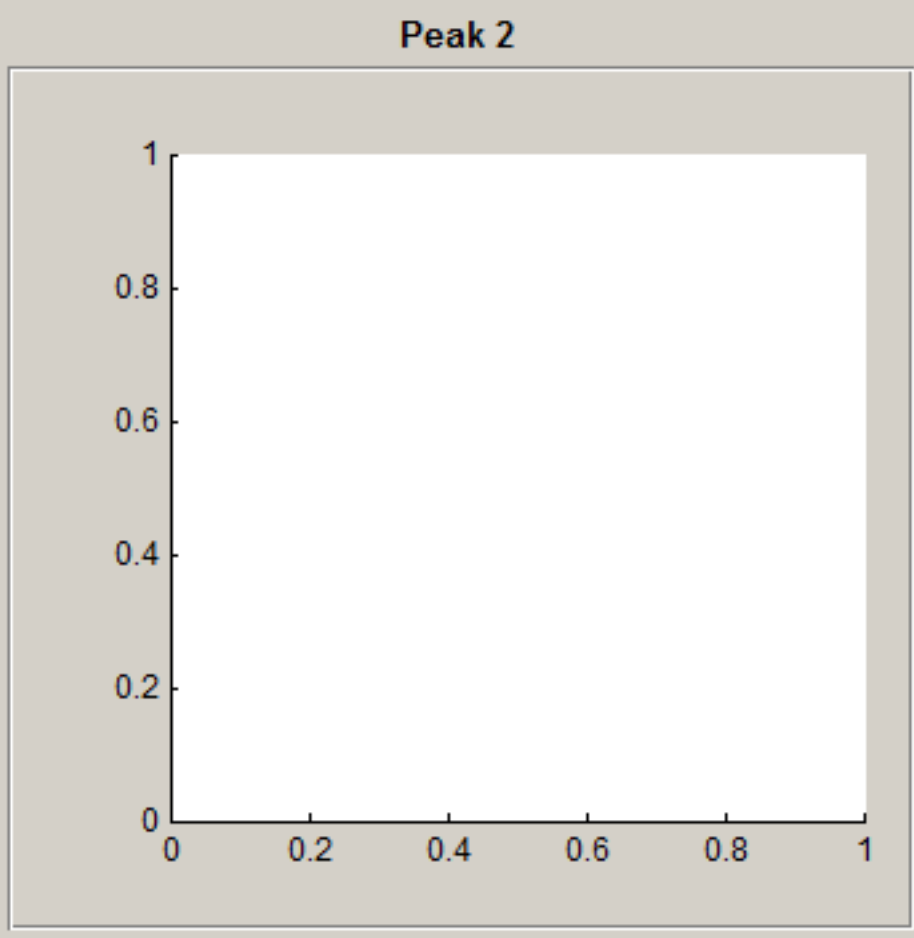
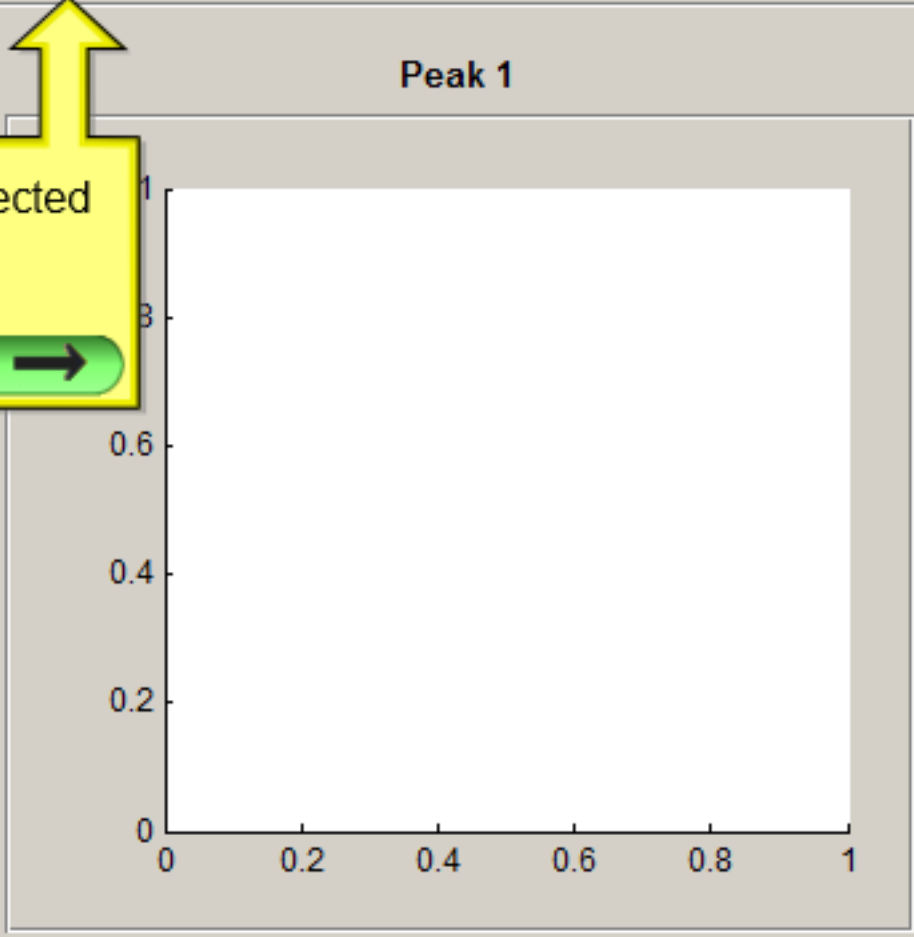
0 0.85 1

Find Correlated Peaks

Peak 1

Peak 2

Correlated with >>>



Export Corr Table

Export Group Figs

Export All Figs

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="ndatat"/>	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="Select Totalcounts..."/>	Name of Samplenames Matrix <input type="text" value="samplegroups ..."/>
--	---	---	--	---

Load Selected Data

Press the 'Load Selected Data' button to load the data into the panel.

Currently Loaded
Data: none
Variables: none
Samplenames: none

Labels to use:

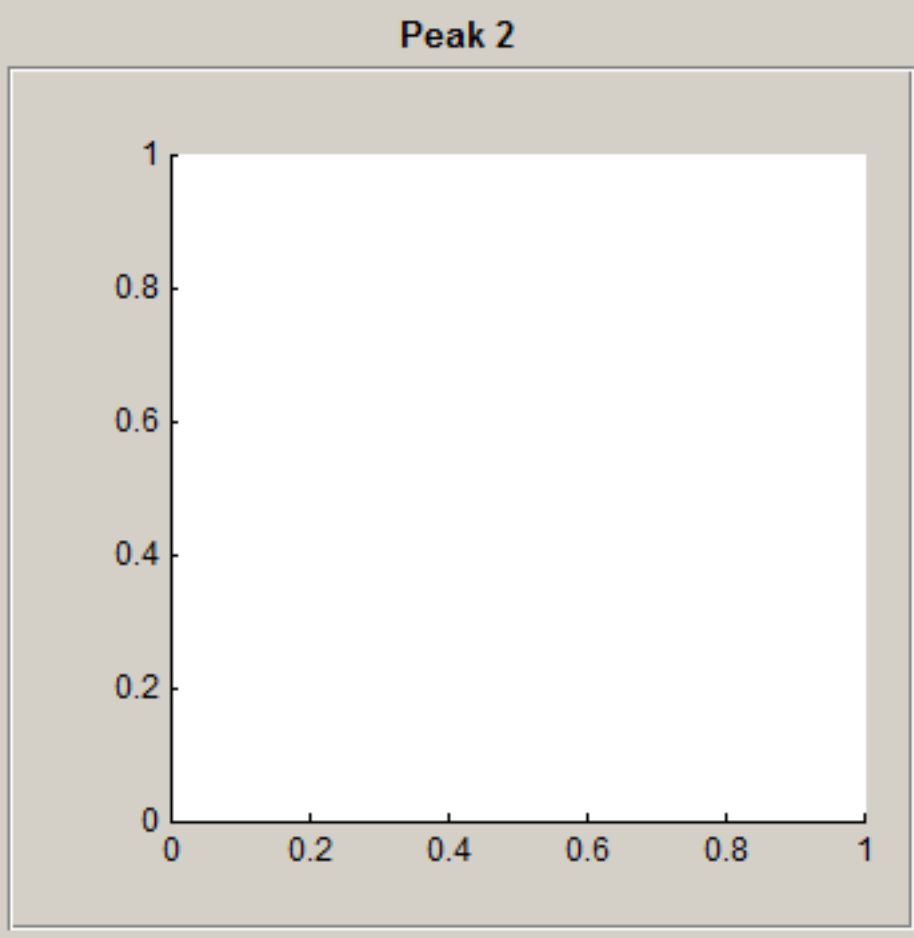
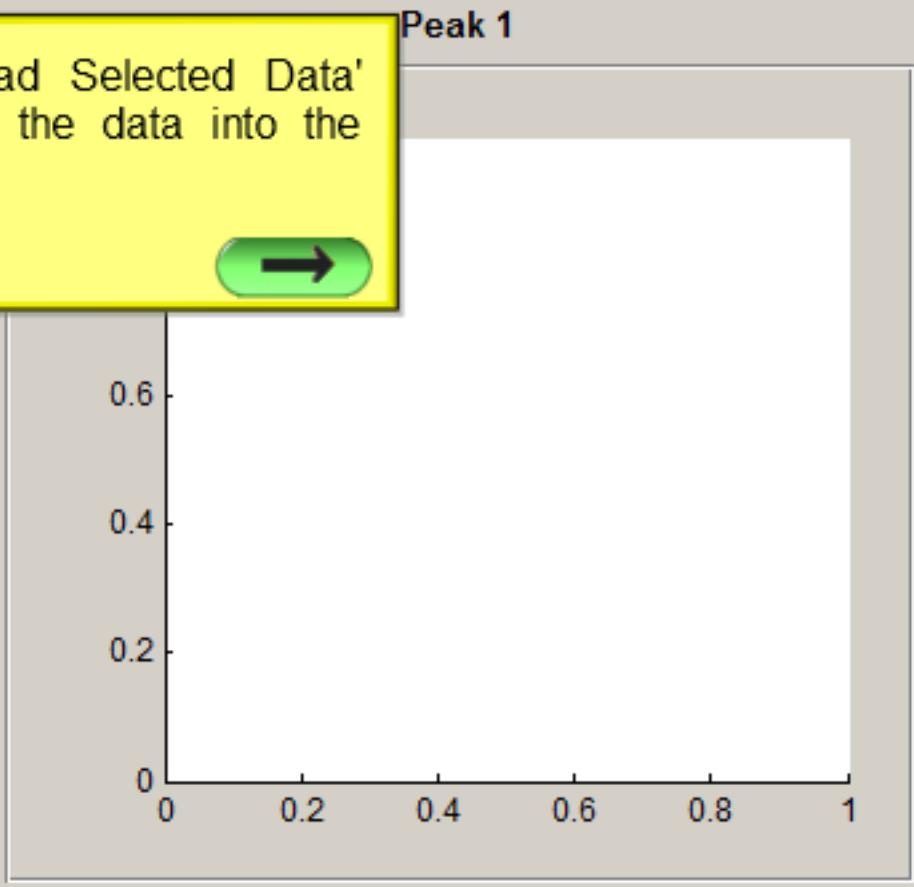
Tolerance value for match (0 to 1)

Find Correlated Peaks

Peak 1

Correlated with >>>

Peak 2



Export Corr Table

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Export All Figs

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="ndatat"/>	<input type="text" value="exactmass"/>	<input type="text" value="filenames"/>	<input type="text" value="Select Totalcounts..."/>	<input type="text" value="samplegroups ..."/>

Load Selected Data

Currently Loaded
Data: **ndatat**
Variables: **exactmass**
Samplenames: **samplegroups**

Labels to use:

Tolerance value for match (0 to 1)
 0.85

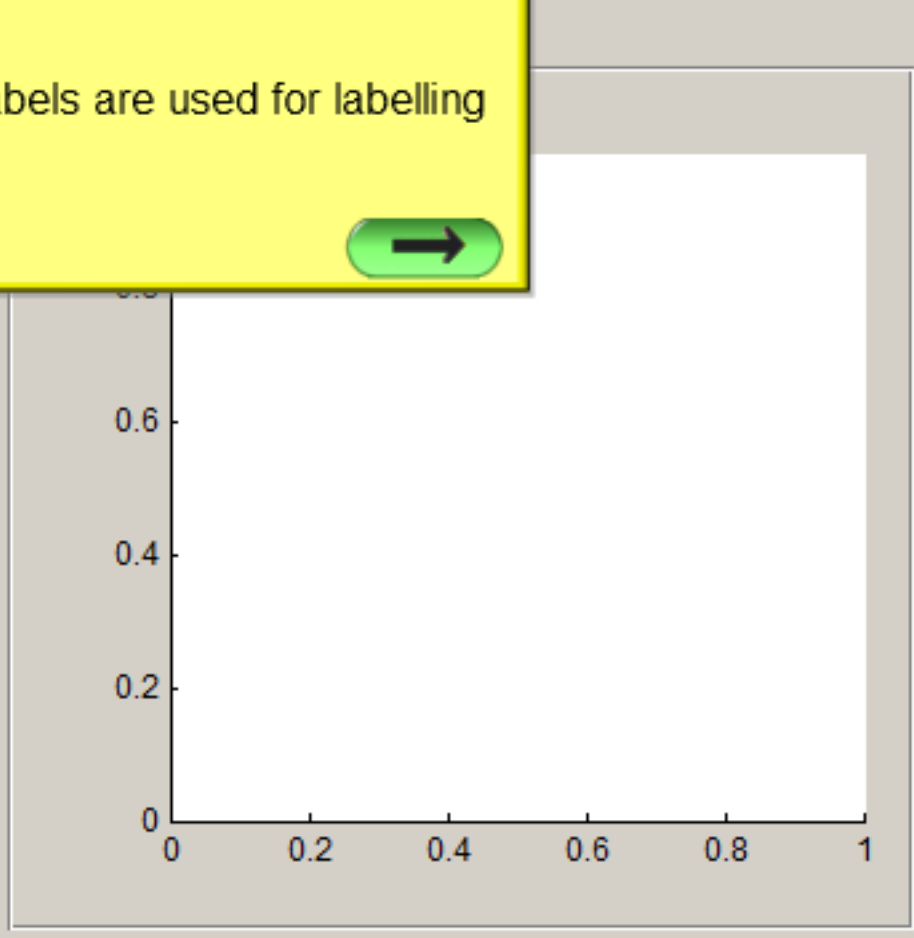
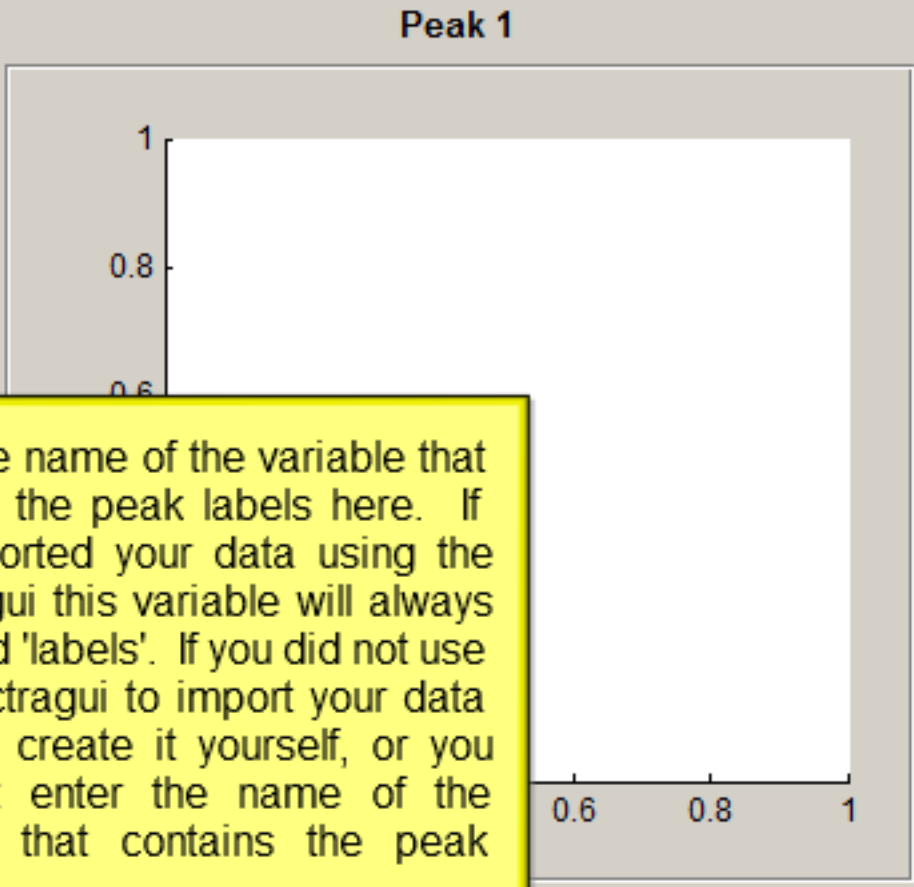
Find Correlated Peaks

Peak 1

Correlated with
>>>

Peak 2

Enter the name of the variable that contains the peak labels here. If you imported your data using the spectragui this variable will always be called 'labels'. If you did not use the spectragui to import your data you can create it yourself, or you can just enter the name of the variable that contains the peak masses. These labels are used for labelling plots.



Export Corr Table

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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:

Load Selected Data

Currently Loaded

Data: **ndatat**

Variables: **exactmass**

Samplenames: **samplegroups**

Labels to use:

Tolerance value for match (0 to 1)

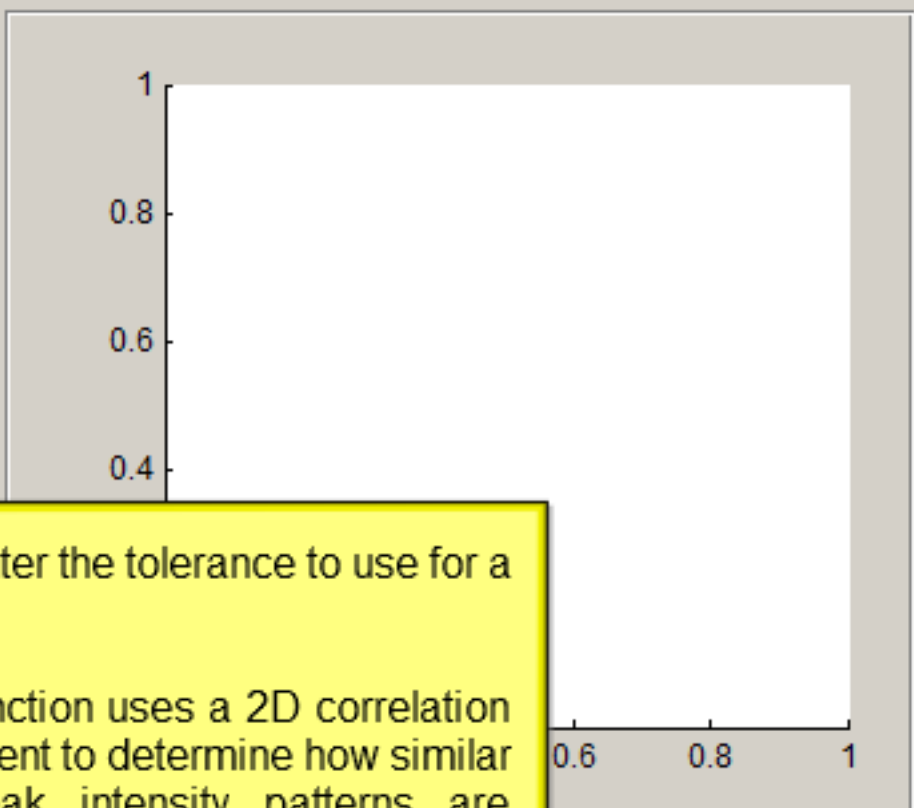
Find Correlated Peaks

Peak 1

Peak 2

Correlated with >>>

Peak 1



Export Corr Table

Export Group Figs

Export All Figs

Close Panel

Next enter the tolerance to use for a match.

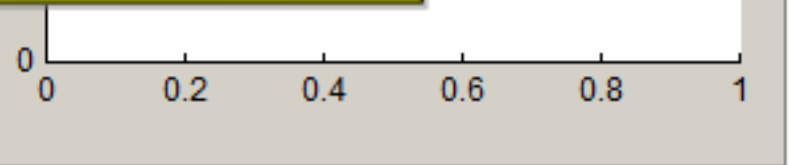
This function uses a 2D correlation coefficient to determine how similar the peak intensity patterns are between peaks.

The tolerance value chooses the lower cut-off for matching peaks. So all peaks with a correlation coefficient above the tolerance will be considered a match.

0 = no match
1 = perfect match

You can enter a value manually or you can use the slider.

← →



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<input type="text" value="ndatat"/>	<input type="text" value="exactmass"/>	<input type="text" value="filenames"/>	<input type="text" value="Select Totalcounts..."/>	<input type="text" value="samplegroups ..."/>

Load Selected Data

Currently Loaded
Data: **ndatat**
Variables: **exactmass**
Samplenames: **samplegroups**

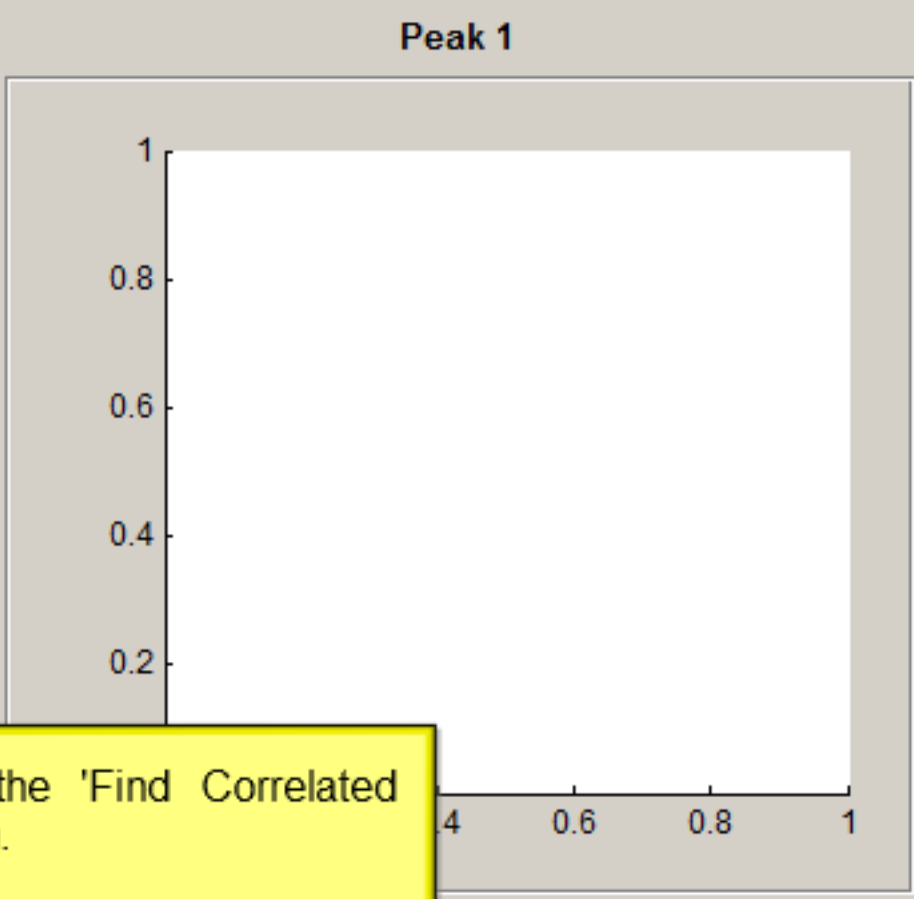
Labels to use:

Tolerance value for match (0 to 1)

0 0.85 1

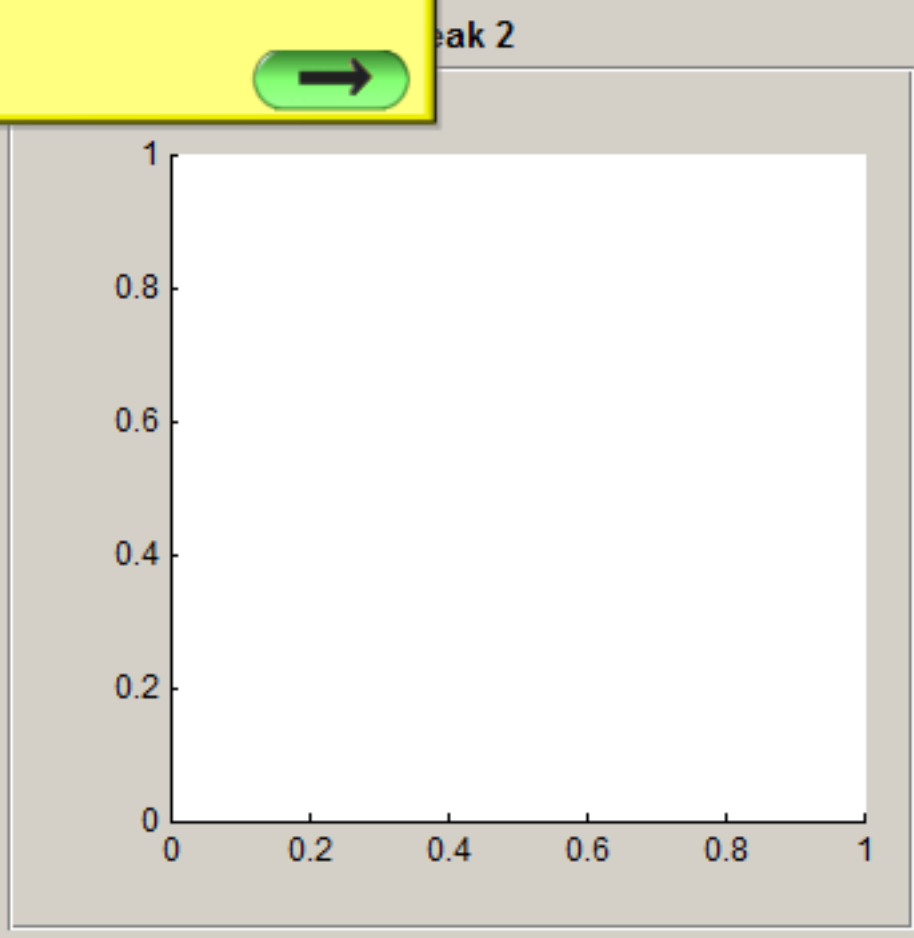
Find Correlated Peaks

Next press the 'Find Correlated Peaks' button.



Peak 1

Pea



Export Corr Table

Export Group Figs

Export All Figs

Close Panel

Correlated with >>>

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

Currently Loaded
Data: **ndatat**
Variables: **exactmass**
Samplenames: **samplegroups**

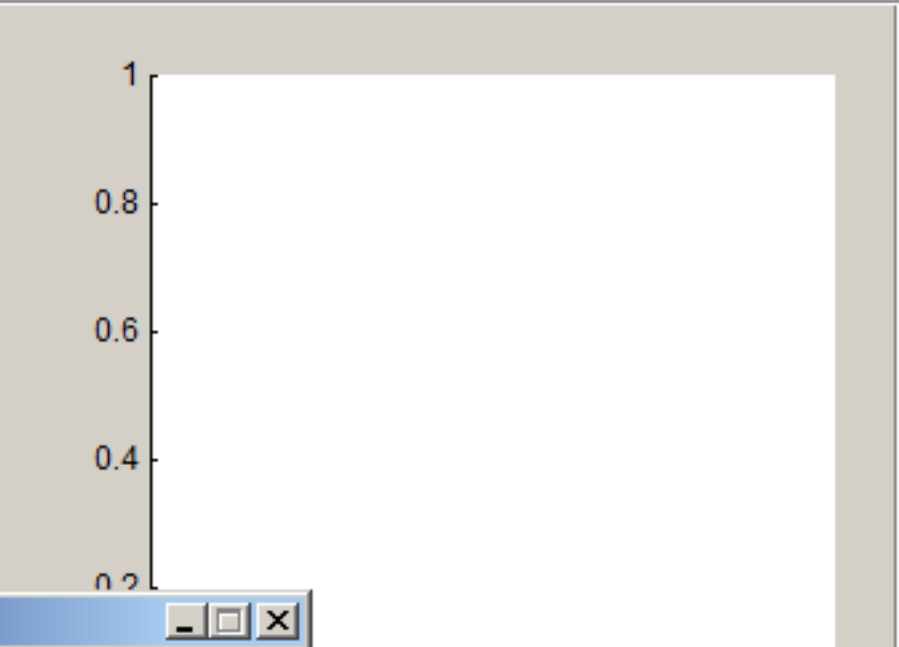
Labels to use:

Tolerance value for match (0 to 1)
 0.85

Find Correlated Peaks

86%
Processing...
 86 %
Estimated time remaining: 00:00:00

Peak 1

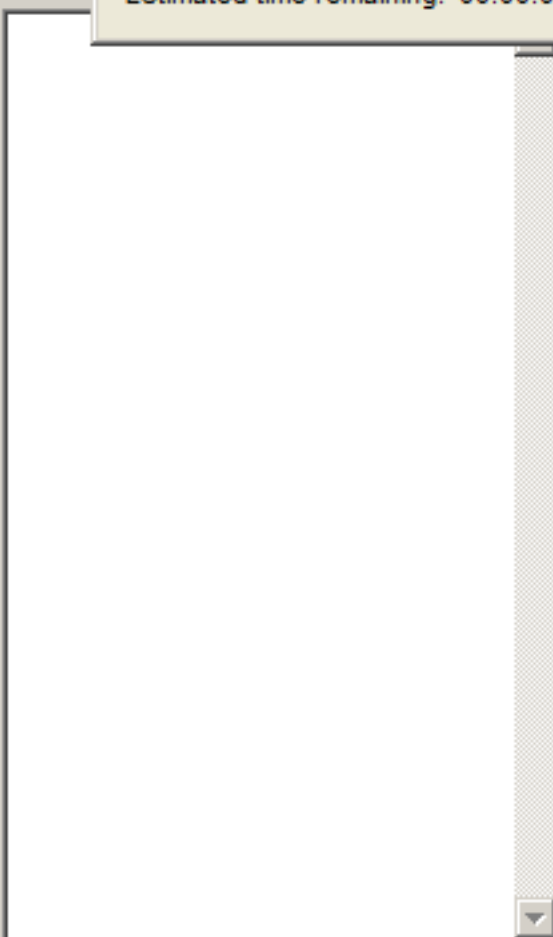


Export Corr Table

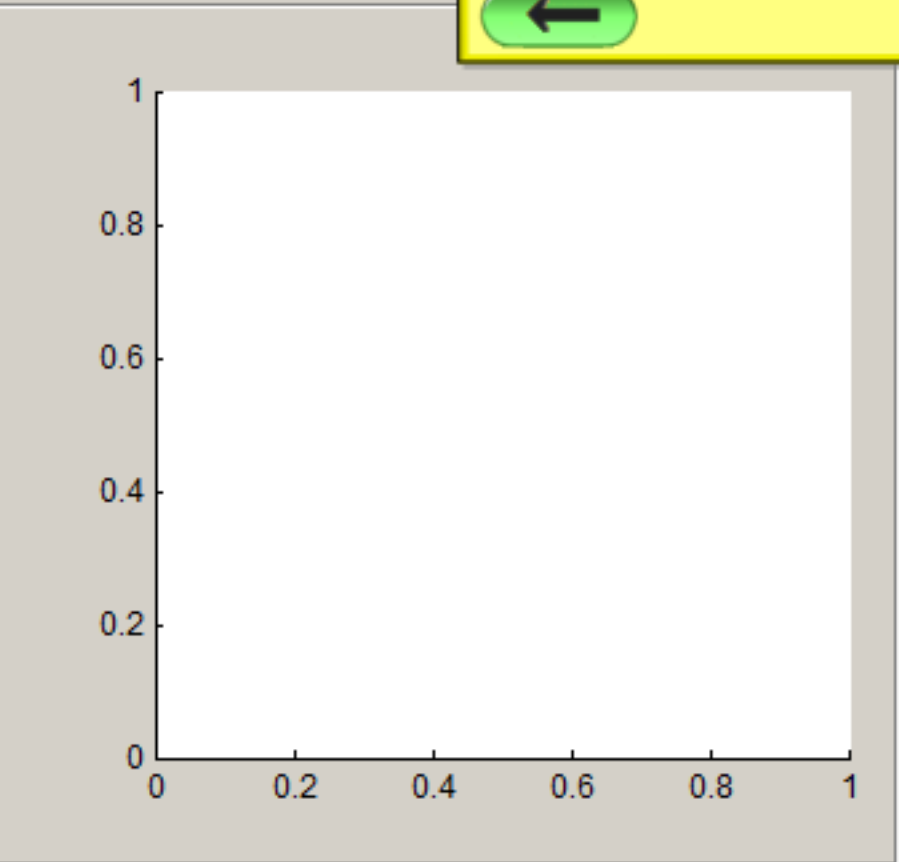
Peak 1



Correlated with
>>>



Peak



A pop-up box will open up showing the progress for the calculations.

Close Panel

Figs

Figs

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:

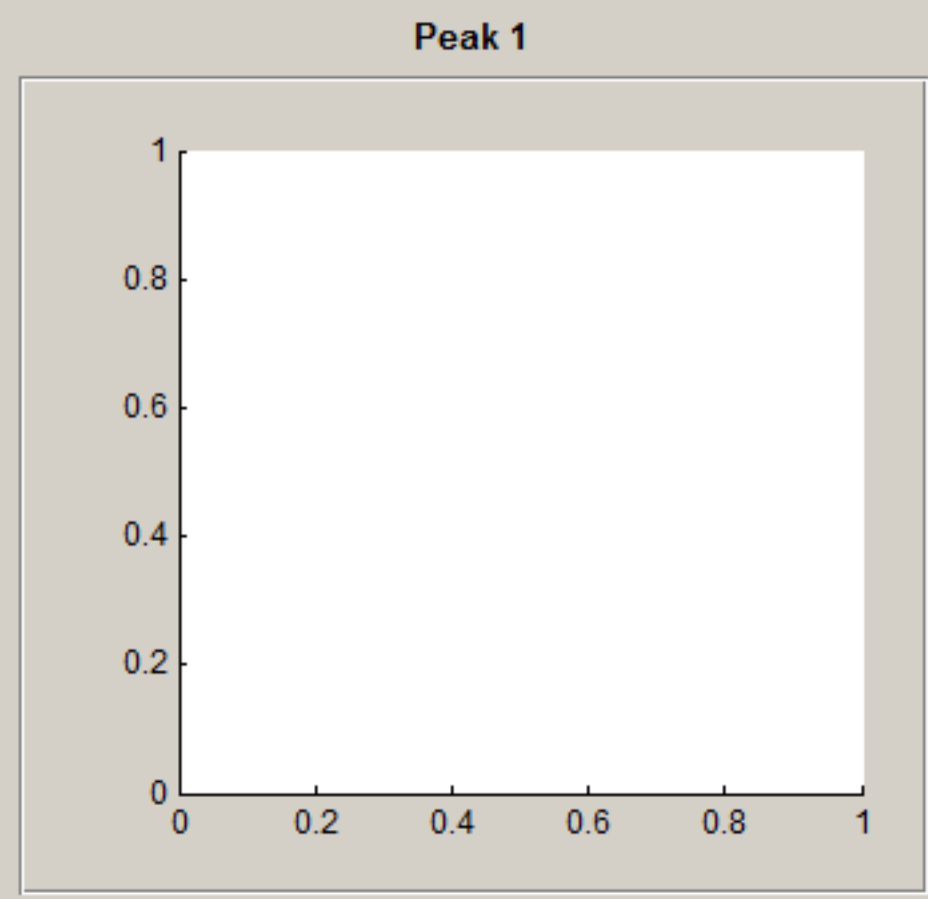
Load Selected Data

Currently Loaded
Data: **ndatat**
Variables: **exactmass**
Samplenames: **samplegroups**

Labels to use:

Tolerance value for match (0 to 1)
 0.85

Find Correlated Peaks



Export Corr Table

Export Group Figs

Export All Figs

Close Panel

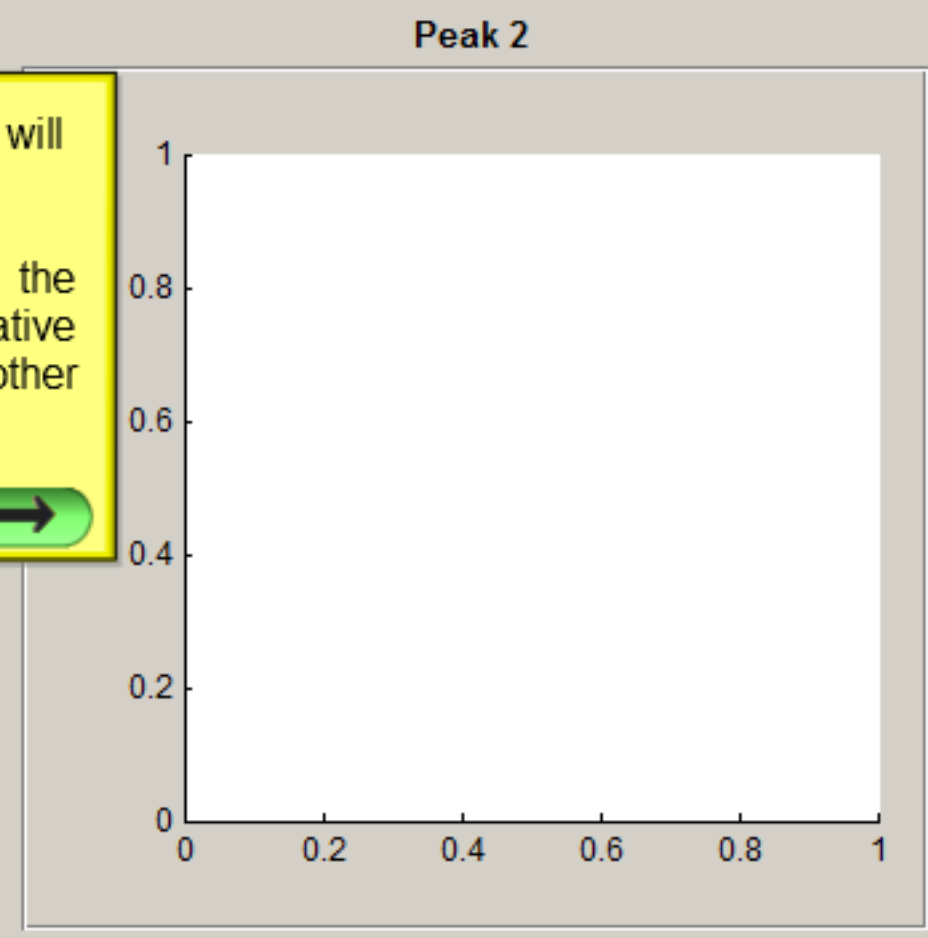
Peak 1	
13.0081	CH
15.9948	O
25.0076	C2H
26.0041	CN
27.0245	C2H3
28.0199	CH2N
29.0032	CHO
31.0184	CH3O
35.9986	C3
37.0065	C3H
41.0128	CH2N
43.0182	C2H3O
43.9892	CO2
44.9969	CHO2
47.9756	POHm
49.0077	C4H
51.0224	C4H3
53.0393	C4H5
56.996	unknown
57.0344	C3H5O
59.9974	unknown

Correlate with >>>

Once it is done a list of peaks will appear in the 'Peak 1' box.
These are the first peaks in the series that showed similar relative peak intensity patterns to other peaks.



Peak 2	
--------	--



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Load Selected Data

Currently Loaded
Data: **ndatat**
Variables: **exactmass**
Samplenames: **samplegroups**

Labels to use:

Tolerance value for match (0 to 1)
 0 0.85 1

Find Correlated Peaks

Peak 1

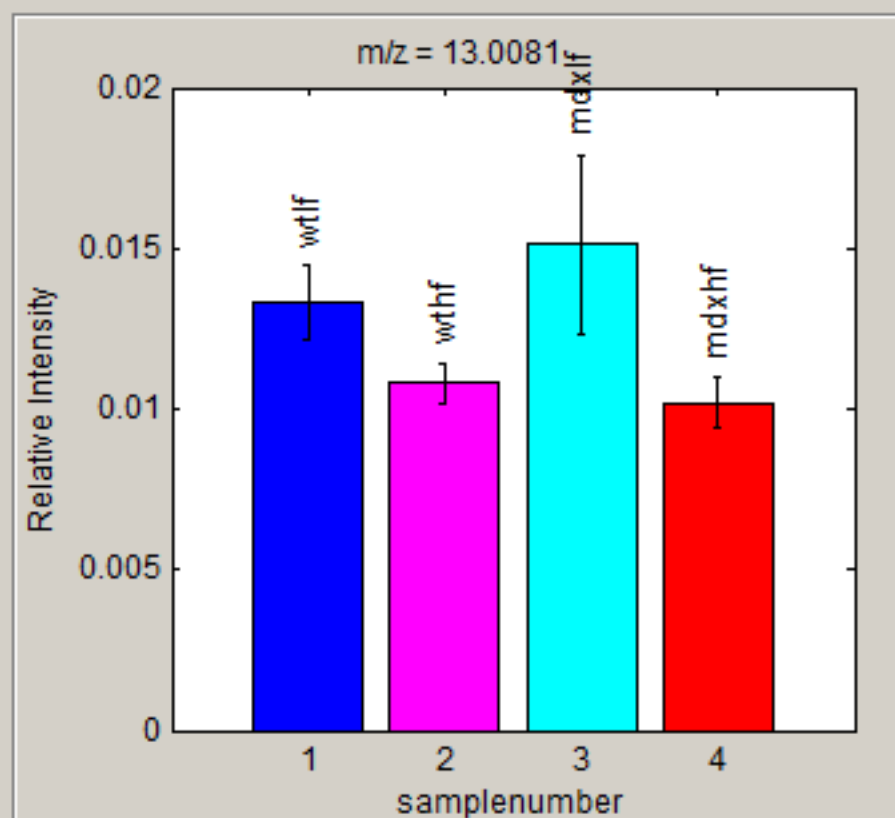
13.0081	CH
15.9948	O
25.0076	C2H
26.0041	CN
27.0245	C2H3
28.0199	CH2N
29.0032	CHO
31.0184	CH3O
35.9986	C3
37.0065	C3H
41.0128	CH2N
43.0182	C2H3O
43.9892	CO2
44.9969	CHO2
47.9756	POHm
49.0077	C4H
51.0224	C4H3
53.0393	C4H5
56.996	unknown
57.0344	C3H5O
59.9974	unknown

Peak 2

30.9721	P
---------	---

Correlated with >>>

Peak 1



Export Corr Table

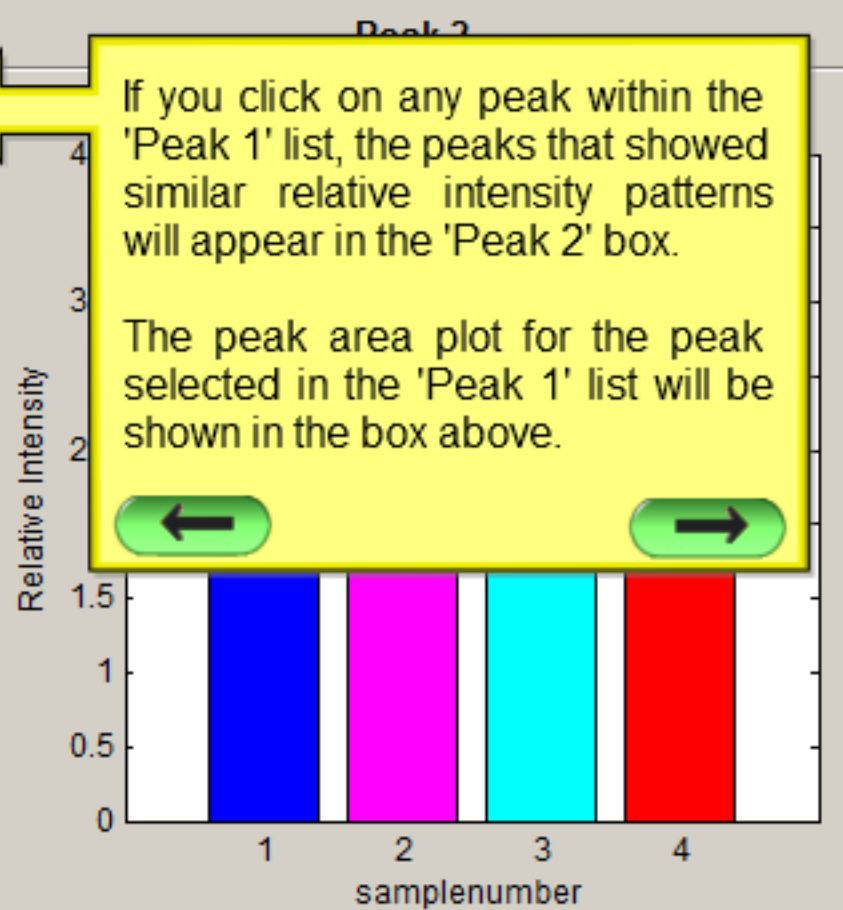
Export Group Figs

Export All Figs

Close Panel

If you click on any peak within the 'Peak 1' list, the peaks that showed similar relative intensity patterns will appear in the 'Peak 2' box.

The peak area plot for the peak selected in the 'Peak 1' list will be shown in the box above.



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Load Selected Data

Currently Loaded
 Data: **ndatat**
 Variables: **exactmass**
 Samplenames: **samplegroups**

Labels to use:

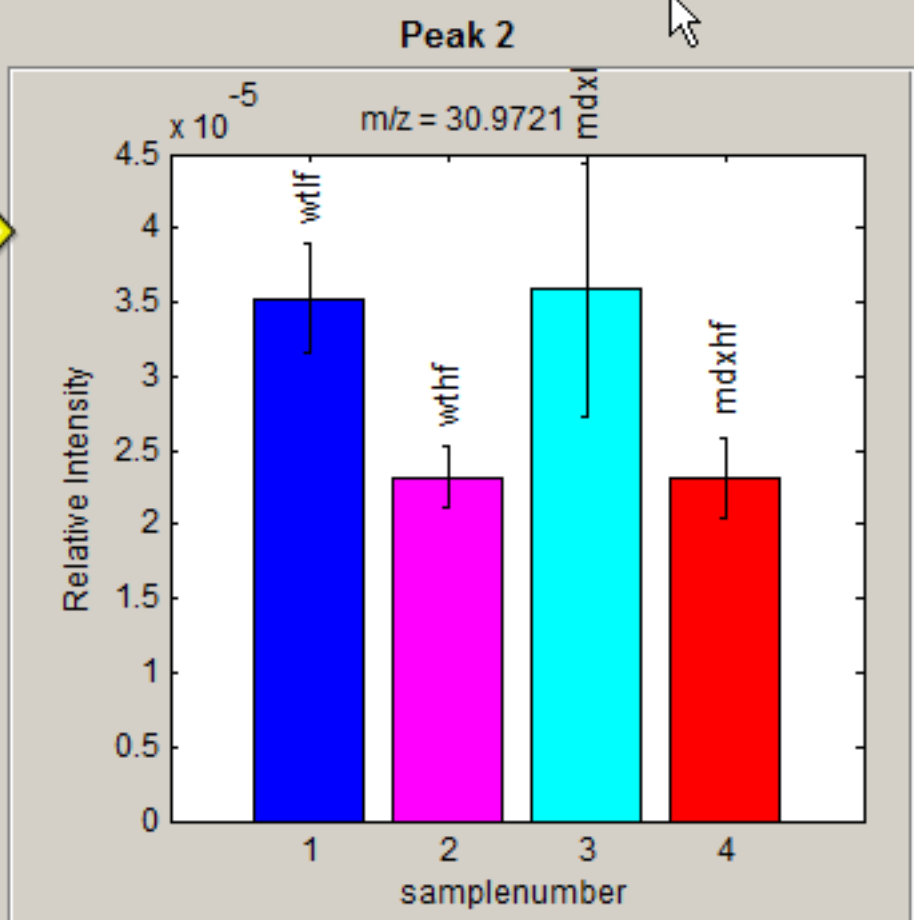
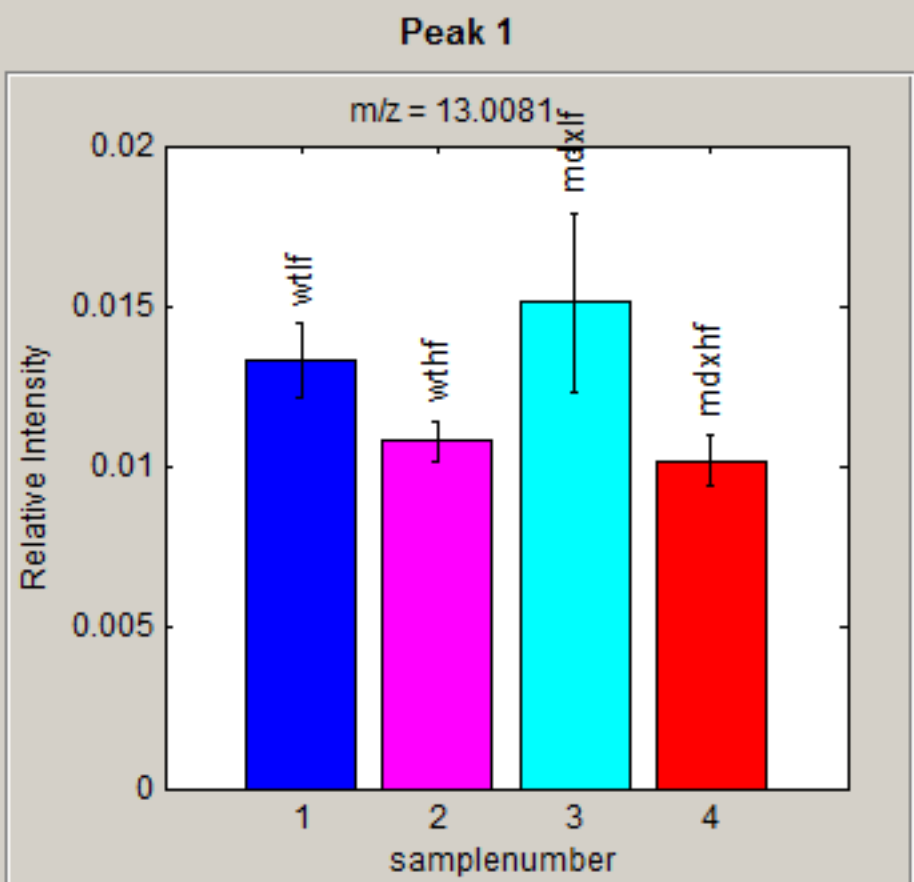
Tolerance value for match (0 to 1)

Find Correlated Peaks

Peak 1	Peak 2
13.0081	30.9721
15.9948	P
25.0076	
26.0041	
27.0245	
28.0199	
29.0032	
31.0184	
35.9986	
37.0065	
41.0128	
43.0182	
43.9892	
44.9969	
47.9756	
49.0077	
51.0224	
53.0393	
56.996	
57.0344	
59.9974	

Clicking on a peak in the 'Peak 2' list will show the peak area plot for the selected peak in the lower box.

As can be seen, the relative intensities of the two peaks follow the same pattern.



Export Corr Table

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Export All Figs

Close 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:

Load Selected Data

Currently Loaded
 Data: **ndatat**
 Variables: **exactmass**
 Samplenames: **samplegroups**

Labels to use:

Tolerance value for match (0 to 1)
 0.85

Find Correlated Peaks

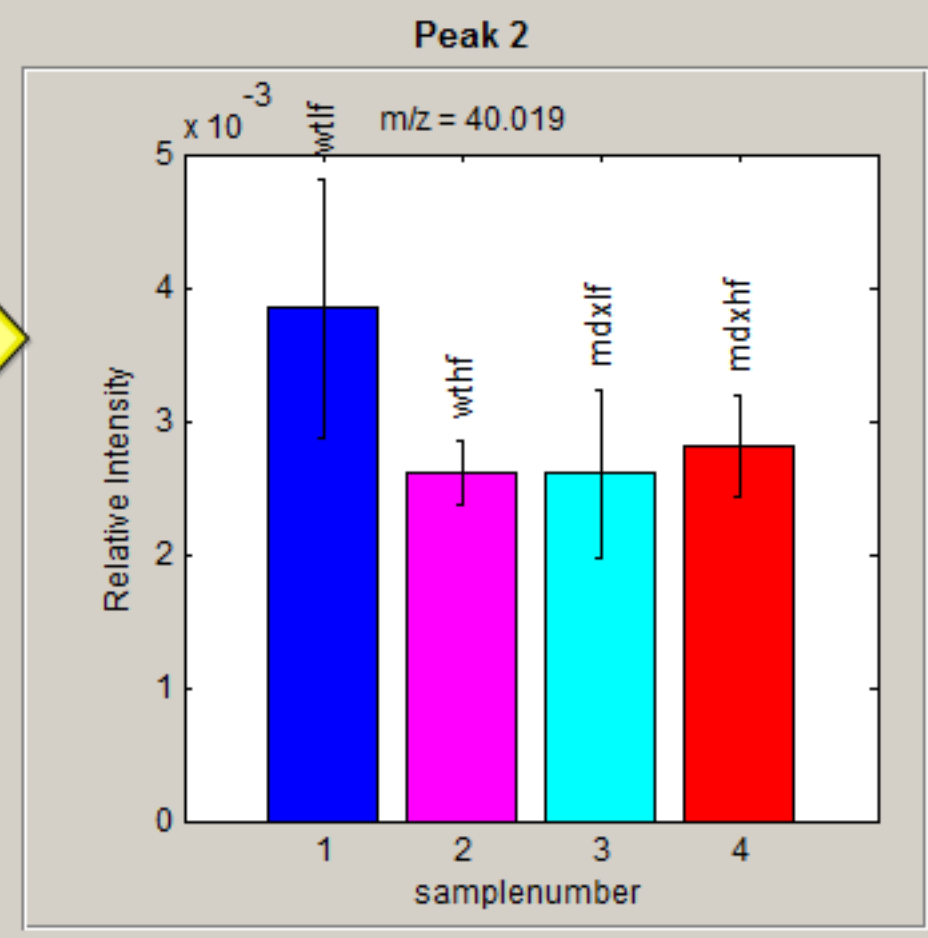
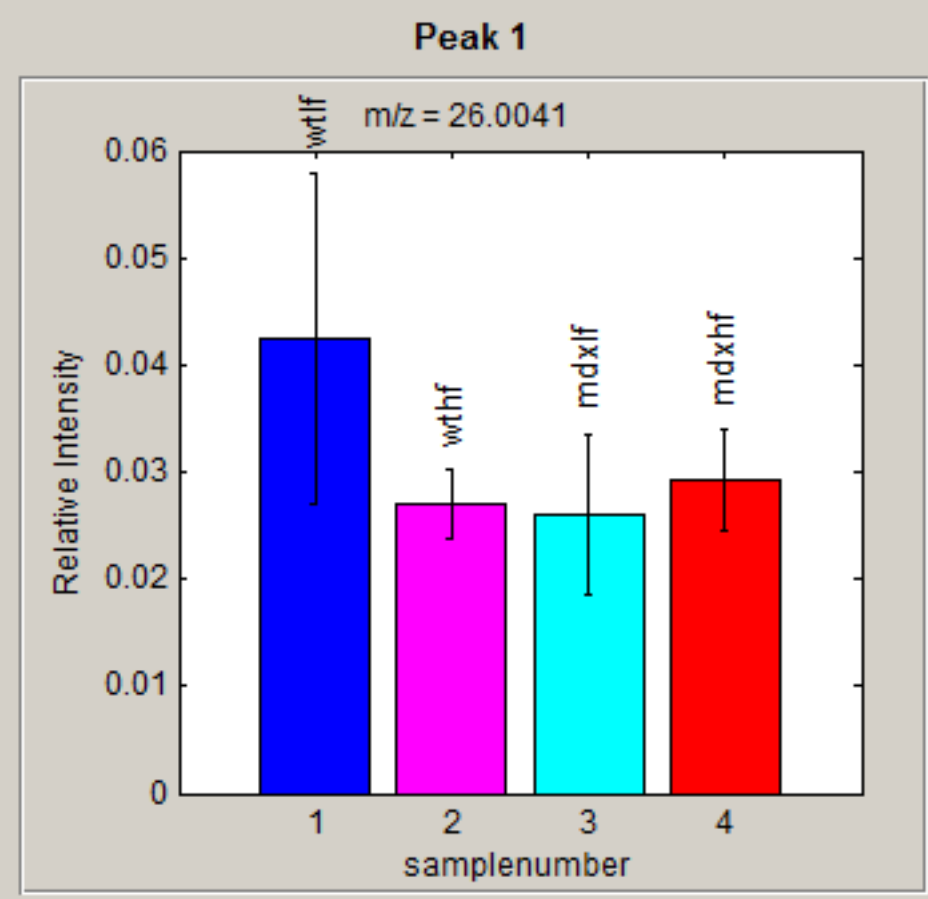
Peak 1

13.0081	CH
15.9948	O
25.0076	C2H
26.0041	CN
27.0245	C2H3
28.0199	CH2N
29.0032	CHO
31.0184	CH3O
35.9986	C3
37.0065	C3H
41.0128	CH2N
43.0182	C2H3O
43.9892	CO2
44.9969	CHO2
47.9756	POHm
49.0077	C4H
51.0224	C4H3
53.0393	C4H5
56.996	unknown
57.0344	C3H5O
59.9974	unknown

Peak 2

28.0199	CH2N
32.98	HS
39.0098	unknown
40.019	C2H2N
41.9992	CNO
44.0149	CH2NO
83.0279	C3H3N2O
84.0121	C3H2NO2m
89.014	C2H3NO2m

This can be seen for other combinations of peaks between the 'Peak 1' and 'Peak 2' boxes. Some matches may not be perfect depending on the tolerance value used.



Export Corr Table

Export Group Figs

Export All Figs

Close 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:

Load Selected Data

Currently Loaded
 Data: **ndatat**
 Variables: **exactmass**
 Samplenames: **samplegroups**

Labels to use:

Tolerance value for match (0 to 1)

Find Correlated Peaks

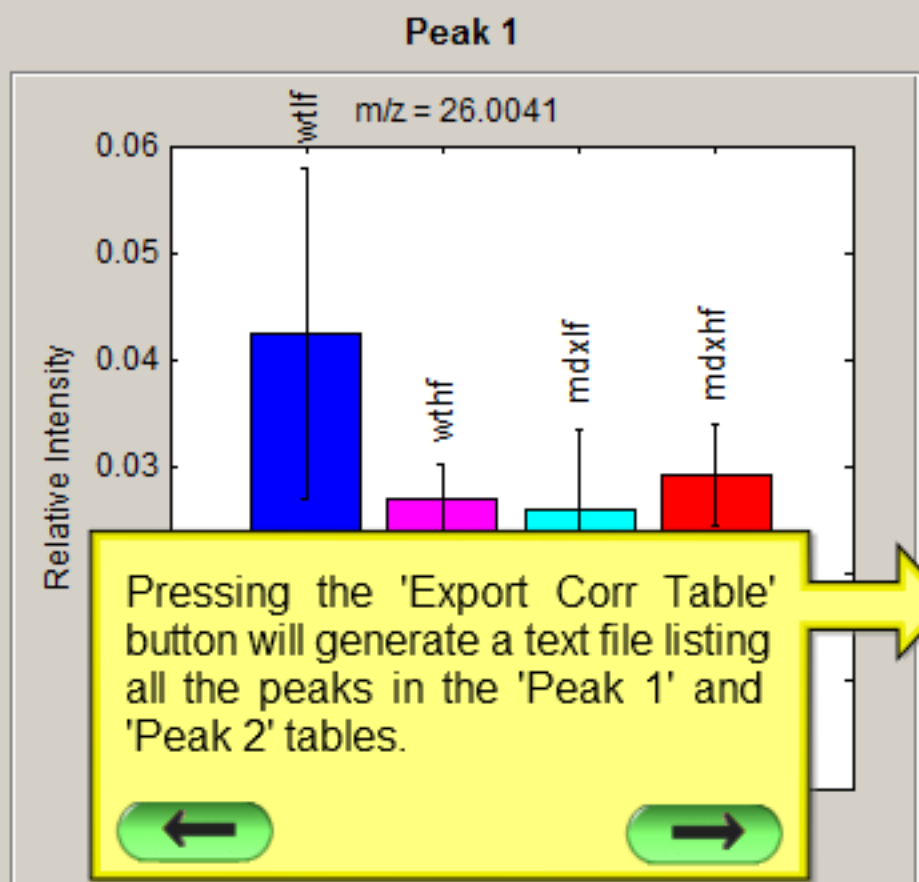
Peak 1

13.0081	CH
15.9948	O
25.0076	C2H
26.0041	CN
27.0245	C2H3
28.0199	CH2N
29.0032	CHO
31.0184	CH3O
35.9986	C3
37.0065	C3H
41.0128	CH2N
43.0182	C2H3O
43.9892	CO2
44.9969	CHO2
47.9756	POHm
49.0077	C4H
51.0224	C4H3
53.0393	C4H5
56.996	unknown
57.0344	C3H5O
59.9974	unknown

Correlated with >>>

Peak 2

28.0199	CH2N
32.98	HS
39.0098	unknown
40.019	C2H2N
41.9992	CNO
44.0149	CH2NO
50.003	C3N
52.019	C3H2N
54.0358	C3H4N
56.0148	C2H2NO
64.0047	C3N2
64.0171	C4H2N
65.0127	C3HN2
65.9977	C3NOm
68.0146	C3H2NO
70.0332	C3H4NO
74.0056	C5N
82.0338	C4H4NO
83.0279	C3H3N2O
84.0121	C3H2NO2m
89.014	C2H3NO2m

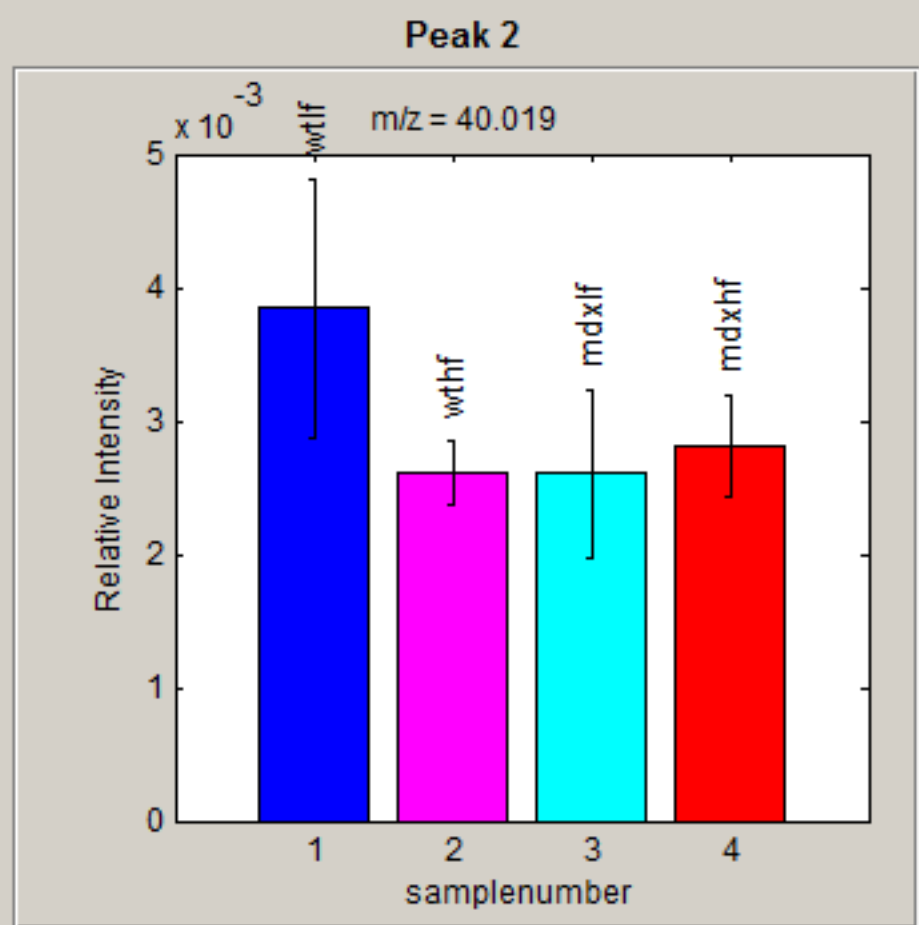


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Load Selected Data

Currently Loaded
Data: **ndatat**
Variables: **exactmass**
Samplenames: **samplegroups**

Labels to use:

Tolerance value for match (0 to 1)

Find Correlated Peaks

Peak 1

13.0081	CH
15.9948	O
25.0076	C2H
26.0041	CN
27.0245	C2H3
28.0199	CH2N
29.0032	CHO
31.0184	CH3O
35.9986	C2
37.0065	C2H2
41.0128	C2H4
43.0182	C2H6
43.9892	C2H5
44.9969	C2H7
47.9756	C2H8
49.0077	C2H9
51.0224	C2H10
53.0393	C4H5
56.996	unknown
57.0344	C3H5O
59.9974	unknown

28.0	
32.9	
39.0	
40.0	
41.9	
44.0	
50.0	
52.0	
54.0	
55.0	
56.0	
57.0	
58.0	
59.0	
60.0	
61.0	
62.0	
63.0	
64.0	
65.0	
66.0	
67.0	
68.0	
69.0	
70.0	
71.0	
72.0	
73.0	
74.0	
75.0	
76.0	
77.0	
78.0	
79.0	
80.0	
81.0	
82.0338	C4H4NO
83.0279	C3H3N2O
84.0121	C3H2NO2m
89.014	C2H3NO2m

Browse For Folder

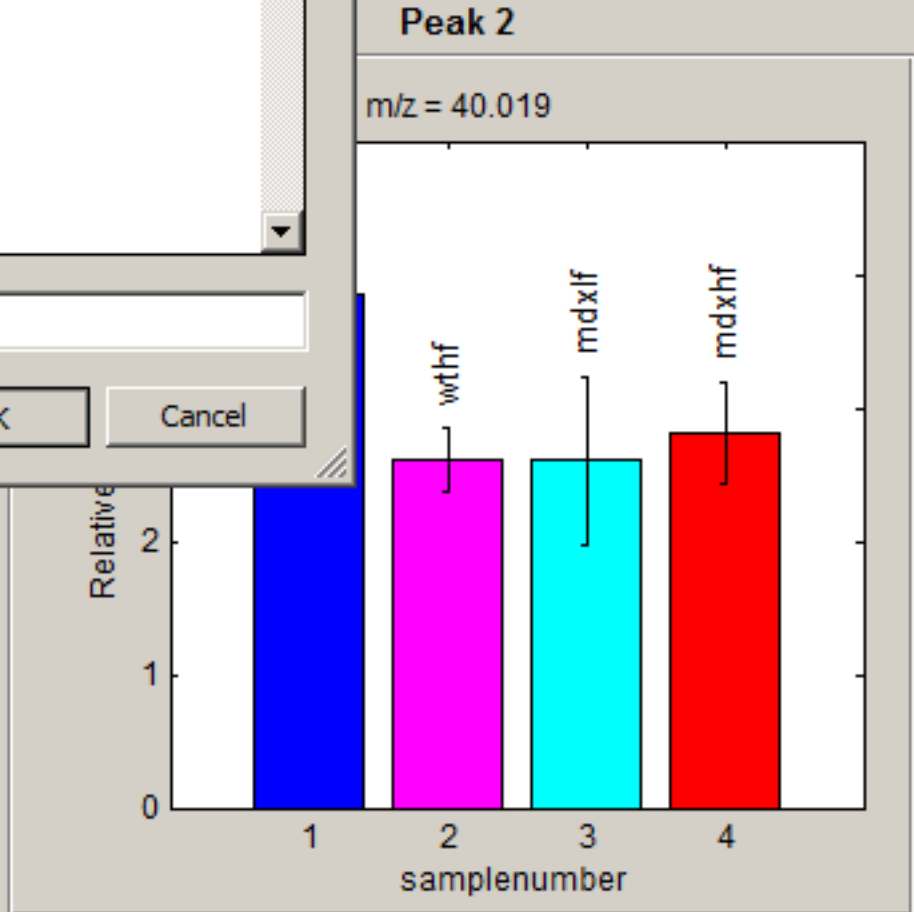
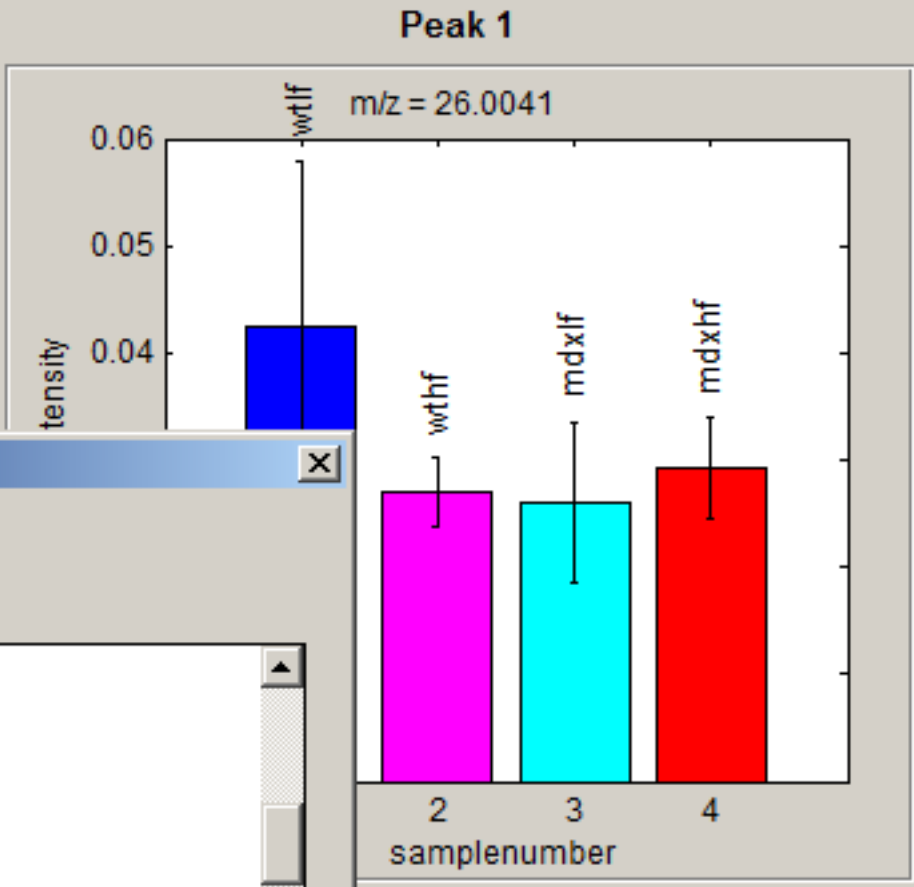
Location to save files

- Favorites
- Links
- Local Settings
- My Documents
 - Bluetooth Folder
 - EndNote
 - MATLAB
 - My Music
 - My Pictures
 - My Tofdata

Folder:

OK Cancel

Choose a location to save the file, and press the 'OK' button.



- Export Corr Table
- Export Group Figs
- Export All Figs
- Close Panel

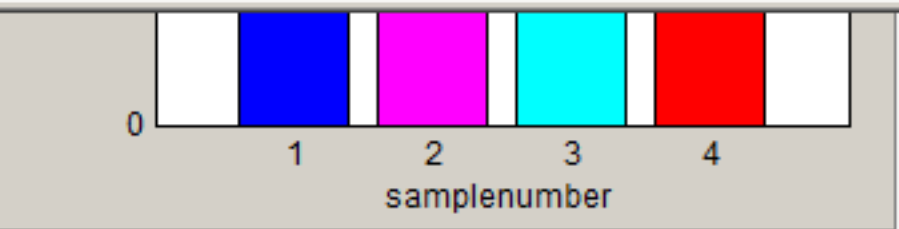
peak1	label1	peak2	label2
13.0081	CH	30.9721	P
15.9948	O	17.0027	OH
15.9948	O	23.9997	CH
25.0076	C2H	35.9986	C3
26.0041	CN	28.0199	CH2N
26.0041	CN	32.98	HS
26.0041	CN	39.0098	unknown
26.0041	CN	40.019	C2H2N
26.0041	CN	41.9992	CNO
26.0041	CN	44.0149	CH2NO
26.0041	CN	50.003	C3N
26.0041	CN	52.019	C3H2N
26.0041	CN	54.0358	C3H4N
26.0041	CN	56.0148	C2H2NO
26.0041	CN	64.0047	C3N2
26.0041	CN	64.0171	C4H2N
26.0041	CN	65.0127	C3HN2
26.0041	CN	65.9977	C3NOM
26.0041	CN	68.0146	C3H2NO
26.0041	CN	70.0332	C3H4NO
26.0041	CN	74.0056	C5N
26.0041	CN	82.0338	C4H4NO
26.0041	CN	83.0279	C3H3N2O
26.0041	CN	84.0121	C3H2NO2m
26.0041	CN	89.014	C2H3NO2m
27.0245	C2H3	41.0019	C2HO
27.0245		43.0182	C2H3O
27.0245		43.9892	CO2
27.0245		44.0102	unknown
27.0245		58.0047	C2H2O2
27.0245		59.0139	C2H3O2
27.0245		78.9676	PO3
28.0184		30.0371	CH4N
28.0184		46.9972	unknown
28.0184		99.0202	unknown
28.0184		111.019	unknown
29.0076		41.0019	C2HO
29.0076		43.0182	C2H3O
29.0076		46.9674	PO
29.0076		53.0011	C3HO
29.0076		55.0184	C3H3O
29.0076		67.0179	C4H3O
29.0076		68.9984	C3HO2
31.0184		39.0229	C3H3
31.0184		41.0019	C2HO
31.0184	CH3O	51.993	C3Om
31.0184	CH3O	53.0011	C3HO
31.0184	CH3O	55.0184	C3H3O
31.0184	CH3O	61.0055	unknown
31.0184	CH3O	67.0179	C4H3O
31.0184	CH3O	73.0076	C6H
35.9986	C3	47.999	C4
35.9986	C3	59.9974	unknown
37.0065	C3H	38.0144	C3H2
37.0065	C3H	39.0229	C3H3

This is what the table looks like. The peak mass and label for each peak in the 'Peak 1' list and 'Peak 2' list is shown.

NOTE: The 'Peak 1' peaks are listed once for each corresponding entry in the 'Peak 2' list. That is why 'Peak 1' peaks are shown multiple times.

53.0393	C4H5
56.996	unknown
57.0344	C3H5O
59.9974	unknown

82.0338	C4H4NO
83.0279	C3H3N2O
84.0121	C3H2NO2m
89.014	C2H3NO2m



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

Currently Loaded
 Data: **ndatat**
 Variables: **exactmass**
 Samplenames: **samplegroups**

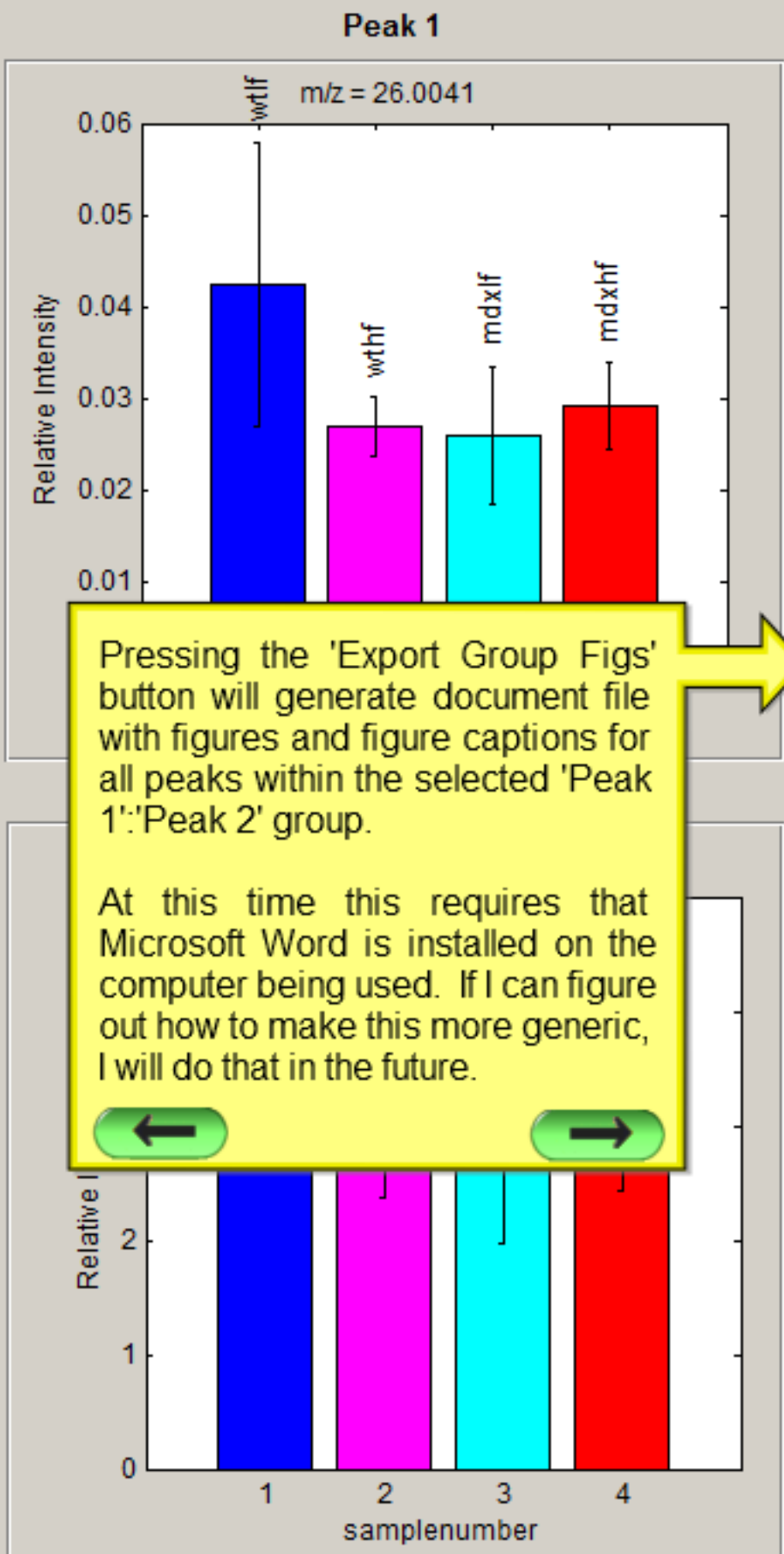
Labels to use:

Tolerance value for match (0 to 1)

Find Correlated Peaks

Peak 1	Peak 2
13.0081	CH
15.9948	O
25.0076	C2H
26.0041	CN
27.0245	C2H3
28.0199	CH2N
29.0032	CHO
31.0184	CH3O
35.9986	C3
37.0065	C3H
41.0128	CH2N
43.0182	C2H3O
43.9892	CO2
44.9969	CHO2
47.9756	POHm
49.0077	C4H
51.0224	C4H3
53.0393	C4H5
56.996	unknown
57.0344	C3H5O
59.9974	unknown
28.0199	CH2N
32.98	HS
39.0098	unknown
40.019	C2H2N
41.9992	CNO
44.0149	CH2NO
50.003	C3N
52.019	C3H2N
54.0358	C3H4N
56.0148	C2H2NO
64.0047	C3N2
64.0171	C4H2N
65.0127	C3HN2
65.9977	C3NOm
68.0146	C3H2NO
70.0332	C3H4NO
74.0056	C5N
82.0338	C4H4NO
83.0279	C3H3N2O
84.0121	C3H2NO2m
89.014	C2H3NO2m

Correlated with >>>



Pressing the 'Export Group Figs' button will generate document file with figures and figure captions for all peaks within the selected 'Peak 1': 'Peak 2' group.

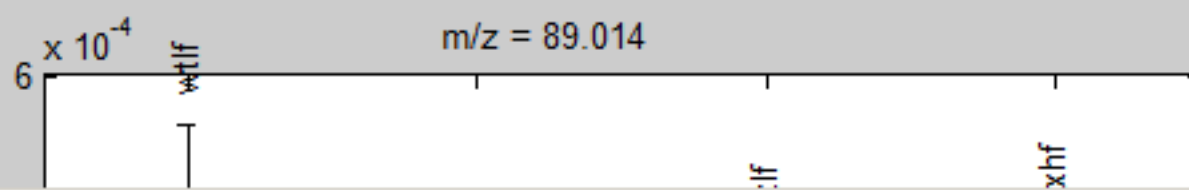
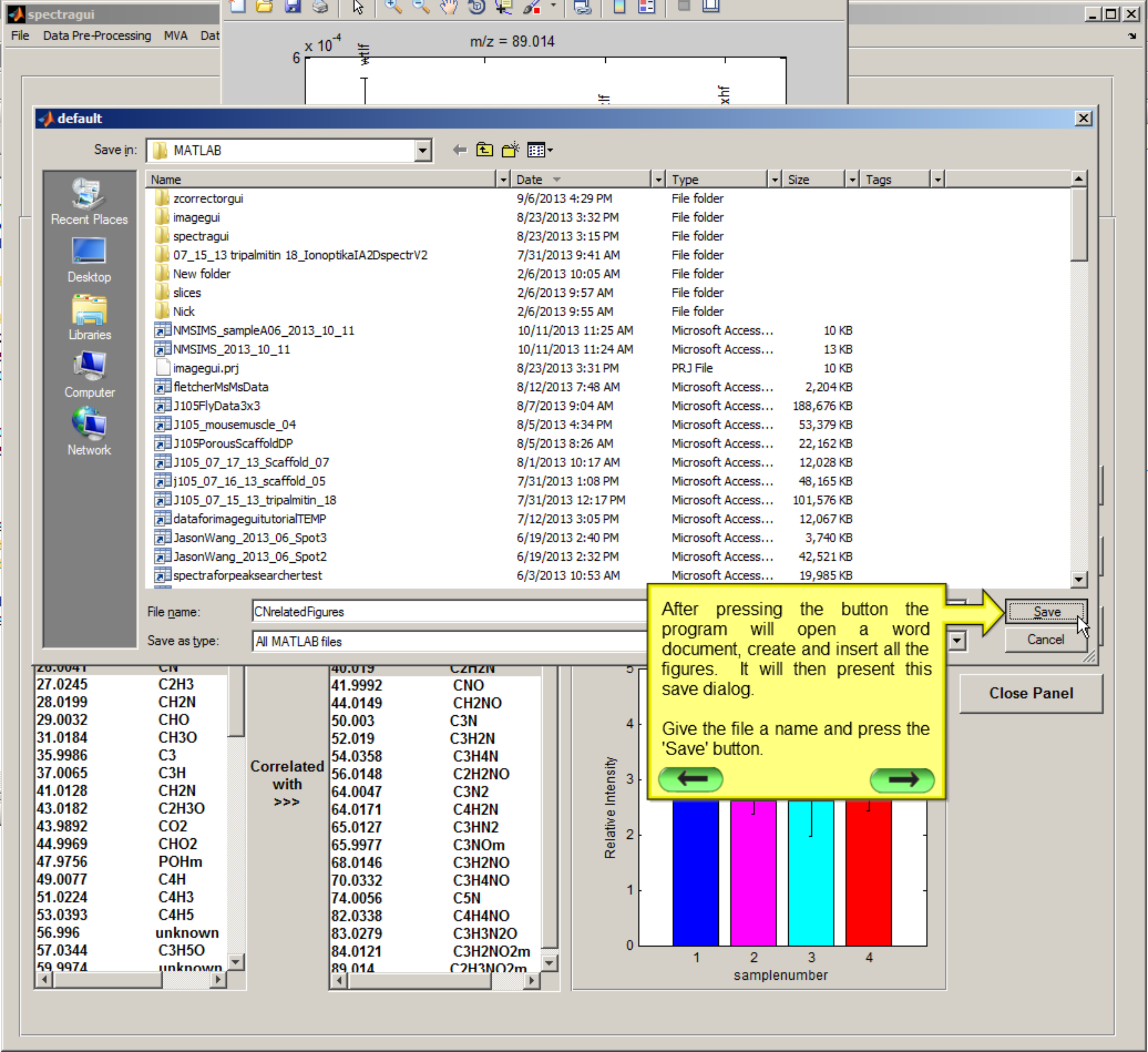
At this time this requires that Microsoft Word is installed on the computer being used. If I can figure out how to make this more generic, I will do that in the future.

Export Corr Table

Export Group Figs

Export All Figs

Close Panel



default

Save in:

Name	Date	Type	Size	Tags
zcorrectorgui	9/6/2013 4:29 PM	File folder		
imagegui	8/23/2013 3:32 PM	File folder		
spectragui	8/23/2013 3:15 PM	File folder		
07_15_13 tripalmitin 18_IonoptikaIA2DspectrV2	7/31/2013 9:41 AM	File folder		
New folder	2/6/2013 10:05 AM	File folder		
slices	2/6/2013 9:57 AM	File folder		
Nick	2/6/2013 9:55 AM	File folder		
NMSIMS_sampleA06_2013_10_11	10/11/2013 11:25 AM	Microsoft Access...	10 KB	
NMSIMS_2013_10_11	10/11/2013 11:24 AM	Microsoft Access...	13 KB	
imagegui.prj	8/23/2013 3:31 PM	PRJ File	10 KB	
fletcherMsMsData	8/12/2013 7:48 AM	Microsoft Access...	2,204 KB	
J105FlyData3x3	8/7/2013 9:04 AM	Microsoft Access...	188,676 KB	
J105_mousemuscle_04	8/5/2013 4:34 PM	Microsoft Access...	53,379 KB	
J105PorousScaffoldDP	8/5/2013 8:26 AM	Microsoft Access...	22,162 KB	
J105_07_17_13_Scaffold_07	8/1/2013 10:17 AM	Microsoft Access...	12,028 KB	
j105_07_16_13_scaffold_05	7/31/2013 1:08 PM	Microsoft Access...	48,165 KB	
J105_07_15_13_tripalmitin_18	7/31/2013 12:17 PM	Microsoft Access...	101,576 KB	
dataforimageguitutorialTEMP	7/12/2013 3:05 PM	Microsoft Access...	12,067 KB	
JasonWang_2013_06_Spot3	6/19/2013 2:40 PM	Microsoft Access...	3,740 KB	
JasonWang_2013_06_Spot2	6/19/2013 2:32 PM	Microsoft Access...	42,521 KB	
spectraforpeaksearchertest	6/3/2013 10:53 AM	Microsoft Access...	19,985 KB	

File name:

Save as type:

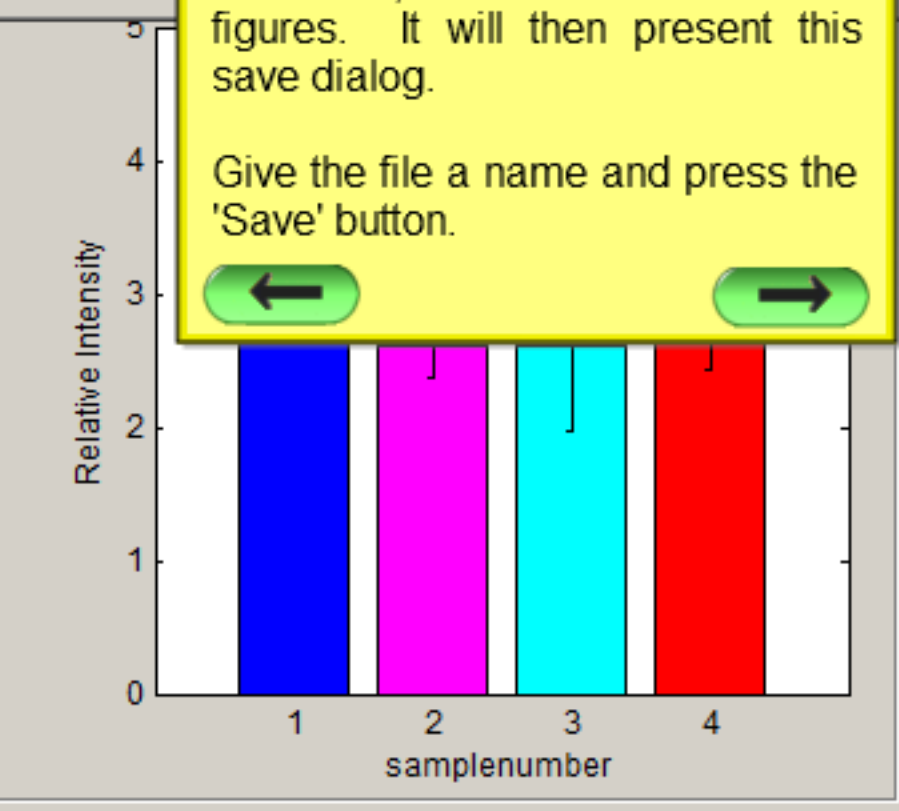
Save Cancel

After pressing the button the program will open a word document, create and insert all the figures. It will then present this save dialog.

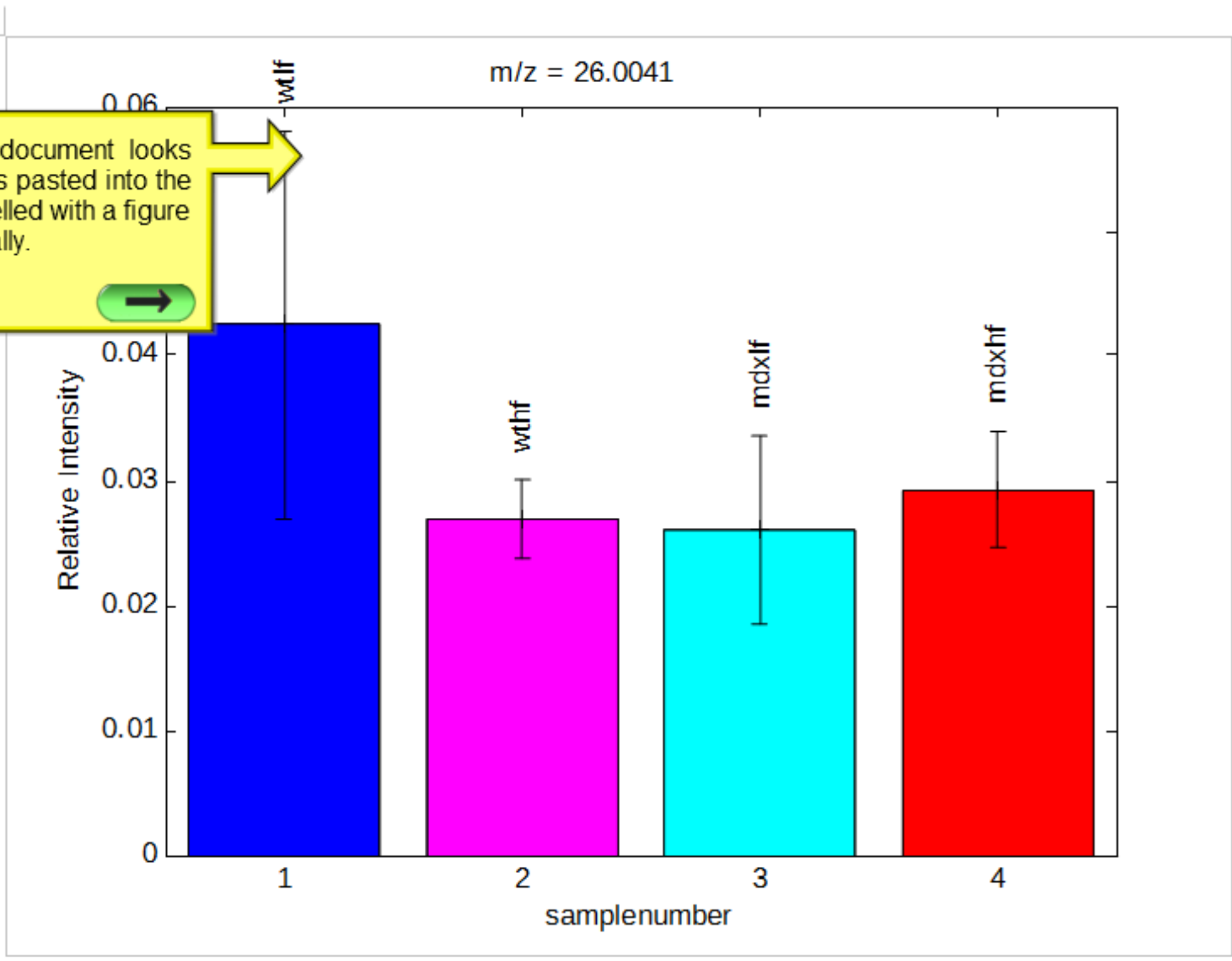
Give the file a name and press the 'Save' button.

Correlated with >>>

20.0041	CN
27.0245	C2H3
28.0199	CH2N
29.0032	CHO
31.0184	CH3O
35.9986	C3
37.0065	C3H
41.0128	CH2N
43.0182	C2H3O
43.9892	CO2
44.9969	CHO2
47.9756	POHm
49.0077	C4H
51.0224	C4H3
53.0393	C4H5
56.996	unknown
57.0344	C3H5O
59.9974	unknown
40.019	C2H2N
41.9992	CNO
44.0149	CH2NO
50.003	C3N
52.019	C3H2N
54.0358	C3H4N
56.0148	C2H2NO
64.0047	C3N2
64.0171	C4H2N
65.0127	C3HN2
65.9977	C3NOm
68.0146	C3H2NO
70.0332	C3H4NO
74.0056	C5N
82.0338	C4H4NO
83.0279	C3H3N2O
84.0121	C3H2NO2m
89.014	C2H3NO2m



Close Panel



This is what the document looks like. Each figure is pasted into the document and labelled with a figure caption automatically.

Figure 1. m/z = 26.0041 (CN)

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

Currently Loaded
 Data: **ndatat**
 Variables: **exactmass**
 Samplenames: **samplegroups**

Labels to use:

Tolerance value for match (0 to 1)
 0.85

Find Correlated Peaks

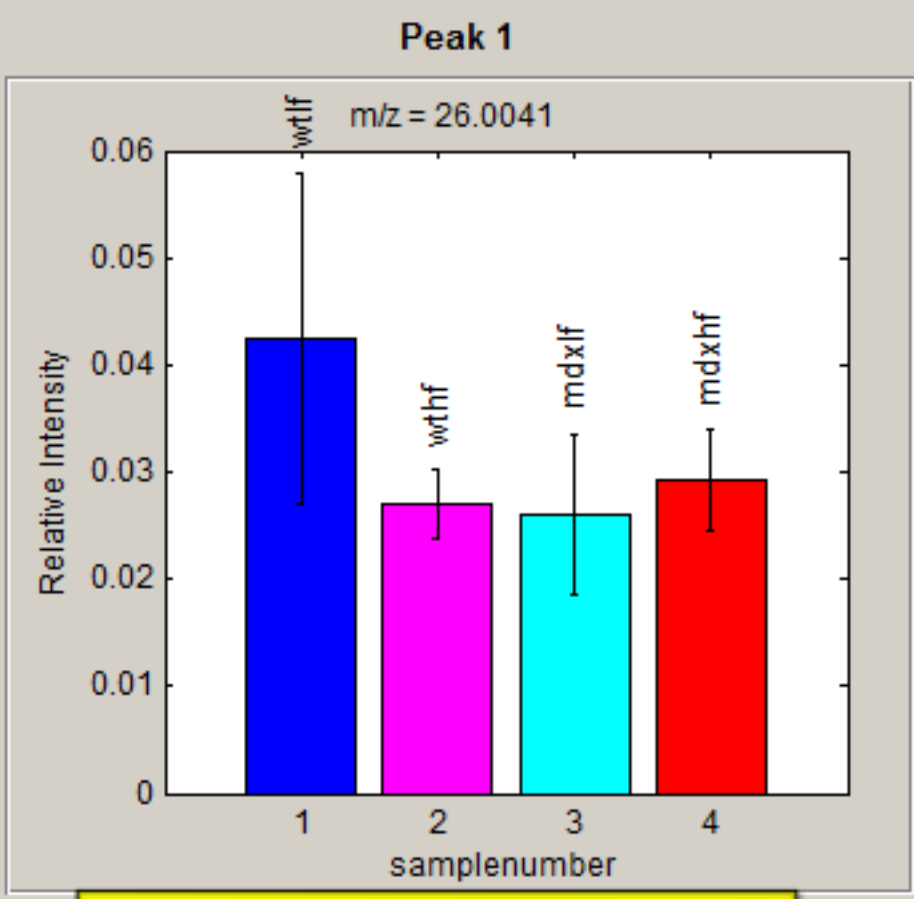
Peak 1

13.0081	CH
15.9948	O
25.0076	C2H
26.0041	CN
27.0245	C2H3
28.0199	CH2N
29.0032	CHO
31.0184	CH3O
35.9986	C3
37.0065	C3H
41.0128	CH2N
43.0182	C2H3O
43.9892	CO2
44.9969	CHO2
47.9756	POHm
49.0077	C4H
51.0224	C4H3
53.0393	C4H5
56.996	unknown
57.0344	C3H5O
59.9974	unknown

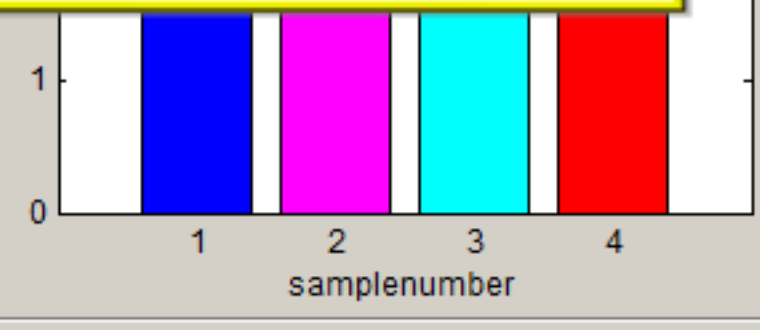
Correlated with >>>

Peak 2

28.0199	CH2N
32.98	HS
39.0098	unknown
40.019	C2H2N
41.9992	CNO
44.0149	CH2NO
50.003	C3N
52.019	C3H2N
54.0358	C3H4N
56.0148	C2H2NO
64.0047	C3N2
64.0171	C4H2N
65.0127	C3HN2
65.9977	C3NOm
68.0146	C3H2NO
70.0332	C3H4NO
74.0056	C5N
82.0338	C4H4NO
83.0279	C3H3N2O
84.0121	C3H2NO2m
89.014	C2H3NO2m



Pressing the 'Export All Figs' button generates a document with figures and figure captions for all peaks in the 'Peak 1': 'Peak 2' lists. Figures are ordered with the first 'Peak 1' figure and then its corresponding 'Peak 2' figures, and then the next 'Peak 1' figure with its corresponding 'Peak 2' figures, and so forth.



Export Corr Table

Export Group Figs

Export All Figs

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

Currently Loaded
 Data: **ndatat**
 Variables: **exactmass**
 Samplenames: **samplegroups**

Labels to use:

Tolerance value for match (0 to 1)

Find Correlated Peaks

Peak 1

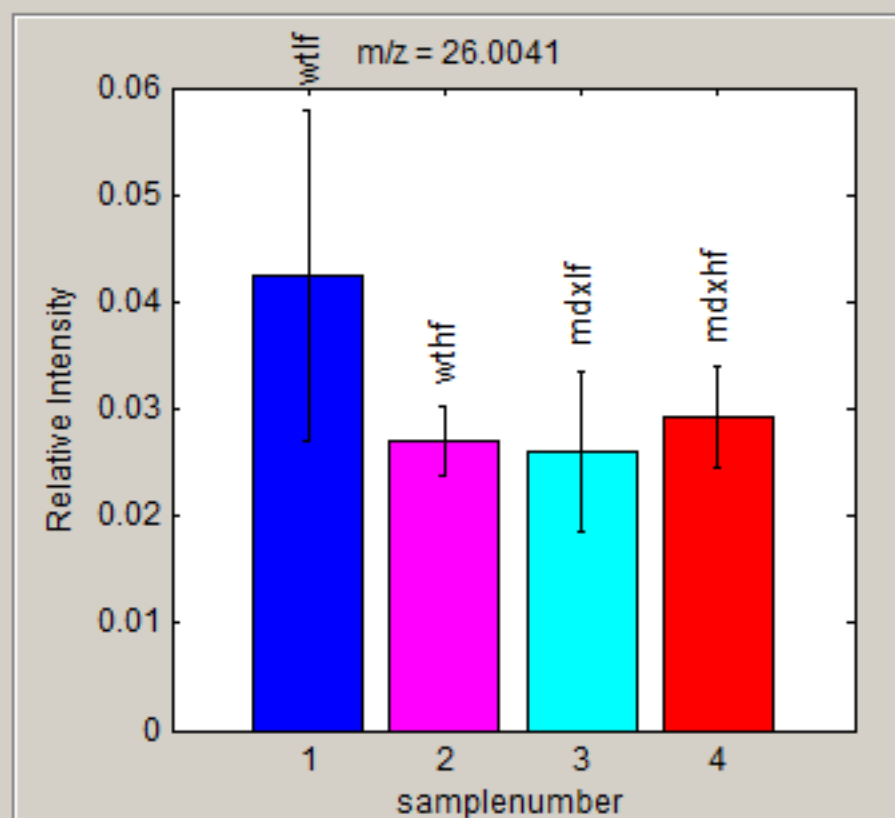
13.0081	CH
15.9948	O
25.0076	C2H
26.0041	CN
27.0245	C2H3
28.0199	CH2N
29.0032	CHO
31.0184	CH3O
35.9986	C3
37.0065	C3H
41.0128	CH2N
43.0182	C2H3O
43.9892	CO2
44.9969	CHO2
47.9756	POHm
49.0077	C4H
51.0224	C4H3
53.0393	C4H5
56.996	unknown
57.0344	C3H5O
59.9974	unknown

Peak 2

28.0199	CH2N
32.98	HS
39.0098	unknown
40.019	C2H2N
41.9992	CNO
44.0149	CH2NO
50.003	C3N
52.019	C3H2N
54.0358	C3H4N
56.0148	C2H2NO
64.0047	C3N2
64.0171	C4H2N
65.0127	C3HN2
65.9977	C3NOm
68.0146	C3H2NO
70.0332	C3H4NO
74.0056	C5N
82.0338	C4H4NO
83.0279	C3H3N2O
84.0121	C3H2NO2m
89.014	C2H3NO2m

Correlated with >>>

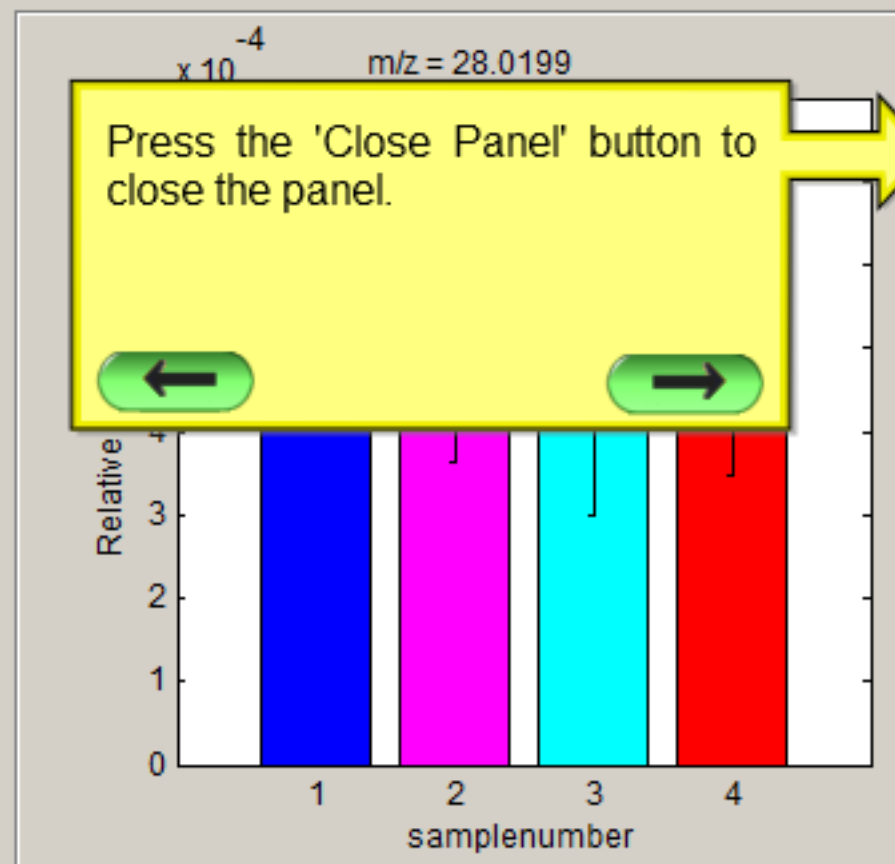
Peak 1



Export Corr Table

Export Group Figs

Peak 2



Export All Figs

Press the 'Close Panel' button to close the panel.

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="ndatat"/>	<input type="text" value="exactmass"/>	<input type="text" value="filenames"/>	<input type="text" value="Select Totalcounts..."/>	<input type="text" value="samplegroups ..."/>

That ends this tutorial. Press the button on the left to go back to the previous step. Press the button on the right to start the tutorial over.

