

1	AUTOMATED SPECTRA EVALUATION REPORT		
2	=====		
3			
4	Filename	S1S1.tdc	S1S
5	=====		
6	# 15.036	4716	
7	# 26.994	18578	
8	# 41.029	27553	
9	# 27.976	7693	
10	# 42.968	12902	8940 12340 13311 7382 10000 441
11	# 73.077	13771	
12	#104.048	9725	
13	#148.968	5158	
14	#104.040	9901	
15	#199.714	594128	

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.



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	AUTOMATED SPECTRA EVALUATION REPORT														
2	=====														
3															
4	Filename	S1S1.tdc	S1S2.tdc	S1S3.tdc	S1S4.tdc	S2S1.tdc	S2S2.tdc	S2S3.tdc							
5	=====														
6	# 15.036	4716	5682	1767	1851	5896	6284	2085							
7	# 26.994	18578	22656	4101	4367	26879	24447	1118							
8	# 41.029	27553	30807	1924											
9	# 27.976	7693	9782	34842											
10	# 42.968	12902	8940	12346											
11	# 73.077	13771	8484	23301											
12	#104.048	9725	3599	1541											
13	#148.968	5158	2082	2306											
14	#104.040	9901	3900	1581											
15	#199.714	594128	606798	294589	3										
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This tutorial will cover how to get data exported from the PHI Job Wizard into the spectragui.

This tutorial assumes you know how to use the PHI software to choose a set of peaks and then export the peak area data using the Job Wizard.

Since I am not a current PHI user, I cannot answer questions about how to use the PHI software.

← →

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	AUTOMATED SPECTRA EVALUATION REPORT														
2	=====														
3															
4	Filename	S1S1.tdc	S1S2.tdc	S1S3.tdc	S1S4.tdc	S2S1.tdc	S2S2.tdc	S2S3.tdc							
5	=====														
6	# 15.036	4716	5682	1767	1851	5896	6284	2085							
7	# 26.994	18578	22656	4101	4367	26879	24447	1118							
8	# 41.029	27553	30807	1924	1996	37265	26520	457							
9	# 27.976	7693	9782	34842	40051	6283	12190	81974							
10	# 42.968	12902	8940	12346	13311	7582	10060	441							
11	# 73.077	13771	8484	23301	24755	11119	31378	967							
12	#104.048	9725	3599	1541	1578	6565	10444	15							
13	#148.968	5158	2082	2306	2326	3727	6265	367							
14	#104.040	9901	3900	1581	1610	6600	10555	25							
15	#199.714	594128	606798	294589	310284	645783	589882	519708							
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The short version of this tutorial is that you need to make this table exported from the Job Wizard ...

← →

F19

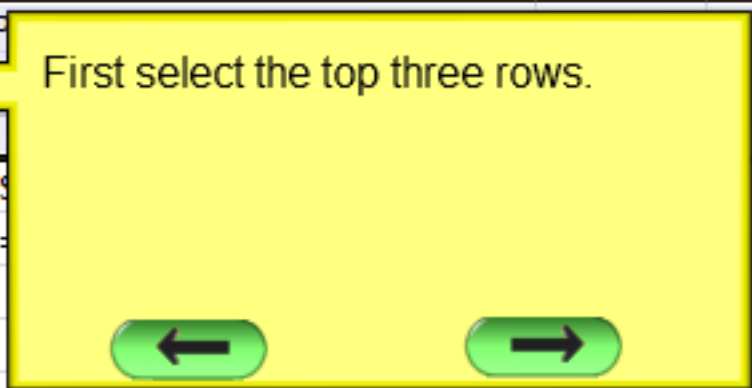
	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	m/z	m/z(nom)	S1S1.tdc	S1S2.tdc	S1S3.tdc	S1S4.tdc	S2S1.tdc	S2S2.tdc	S2S3.tdc					
2	15.04	15	4716	5682	1767	1851	5896	6284	2085					
3	26.99	27	18578	22656	4101	4367	26879	24447	1118					
4	41.03	41	27553	30807	1924	1996	37265	26520	457					
5	27.98	28	7693	9782	34842	40051	6283	12190	81974					
6	42.97	43	12902	8940	12346	13311	7582	10060	441					
7	73.08	73	13771	8484	23301	24755	11119	31378	967					
8	104.05	104	9725	3599	1541	1578	6565	10444	15					
9	148.97	149	5158	2082	2306	2326	3727	6265	367					
10	104.04	104	9901	3900	1581	1610	6600	10555	25					
11	Spectrum	Total	594128	606798	294589	310284	645783	589882	519708					
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Look like this.

If you can do this on your own, you can skip ahead in the tutorial. Here ->

If not, continue on...

First select the top three rows.



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	AUTOMATED SP														
2															
3															
4	Filename	S19				S1.tdc	S2S2.tdc	S2S3.tdc							
5															
6	# 15.036					5896	6284	2085							
7	# 26.994					26879	24447	1118							
8	# 41.029	27553	30807	1924	1996	37265	26520	457							
9	# 27.976	7693	9782	34842	40051	6283	12190	81974							
10	# 42.968	12902	8940	12346	13311	7582	10060	441							
11	# 73.077	13771	8484	23301	24755	11119	31378	967							
12	#104.048	9725	3599	1541	1578	6565	10444	15							
13	#148.968	5158	2082	2306	2326	3727	6265	367							
14	#104.040	9901	3900	1581	1610	6600	10555	25							
15	#199.714	594128	606798	294589	310284	645783	589882	519708							
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	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	Filename	S1S1				S1S1.tdc	S2S2.tdc	S2S3.tdc							
2															
3	# 15.036					5896	6284	2085							
4	# 26.994					26879	24447	1118							
5	# 41.029					37265	26520	457							
6	# 27.976					6283	12190	81974							
7	# 42.968					7582	10060	441							
8	# 73.077	13771	8484	23301	24755	11119	31378	967							
9	#104.048	9725	3599	1541	1578	6565	10444	15							
10	#148.968	5158	2082	2306	2326	3727	6265	367							
11	#104.040	9901	3900	1581	1610	6600	10555	25							
12	#199.714	594128	606798	294589	310284	645783	589882	519708							
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Now do the same with this row (now #2).

← →

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	Filename	S1S1.tdc	S1S2.tdc	S1S3.tdc	S1S4.tdc	S2S1.tdc	S2S2.tdc	S2S3.tdc							
2	# 15.036	4716	5682	1767	1851	5896	6284	2085							
3	# 26.994	18578	22656	4101	4367	26879	24447	1118							
4	# 41.029	27553					26520	457							
5	# 27.976						12190	81974							
6	# 42.968	12902					10060	441							
7	# 73.077	13771					31378	967							
8	#104.048	9725					10444	15							
9	#148.968	5158					6265	367							
10	#104.040	9901					10555	25							
11	#199.7	594128	606798	294589	310284	645783	589882	519708							
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Now select all of the peak masses and do a find and replace to get rid of the '#' symbols.

Find and Replace [?] [X]

Find Replace

Find what: #

Replace with:

Replace All Replace Find All Find Next

To do this bring up the 'Find and Replace' dialog and enter # in the 'Find what' field. Leave the 'Replace with' field blank and press the 'Replace All' button.

← →

8	#104.048	9725	3599	1541					
9	#148.968	5158	2082	2306	2326	3727	6265	367	
10	#104.040	9901	3900	1581	1610	6600	10555	25	
11	#199.714	594128	606798	294589	310284	645783	589882	519708	

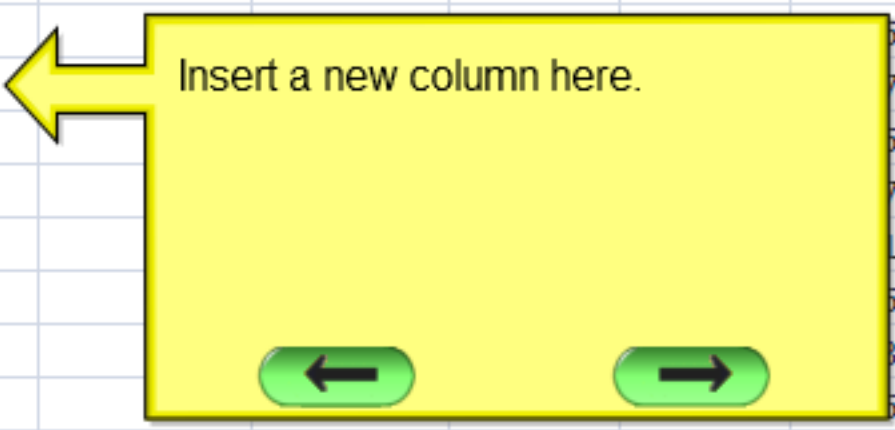
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	m/z	S1	tdc				S2S2.tdc	S2S3.tdc							
2	15.036						6284	2085							
3	26.994	18					24447	1118							
4	41.029	27					26520	457							
5	27.976	7					12190	81974							
6	42.968	12					10060	441							
7	73.077	13					31378	967							
8	104.048	9725	3599	1541	1578	6565	10444	15							
9	148.968	5158	2082	2306	2326	3727	6265	367							
10	104.04	9901	3900	1581	1610	6600	10555	25							
11	199.714	594128	606798	294589	310284	645783	589882	519708							
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Now replace the text of the first cell with 'm/z'.

← →

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	m/z		1.tdc	S1S2.tdc	S1S3.tdc	S1S4.tdc	S2S1.tdc	S2S2.tdc	S2S3.tdc					
2	15.036		4716	5682	1767	1851	5896	6284	2085					
3	26.994						879	24447	1118					
4	41.029						7265	26520	457					
5	27.976						5283	12190	81974					
6	42.968						7582	10060	441					
7	73.077						119	31378	967					
8	104.048						5565	10444	15					
9	148.968						727	6265	367					
10	104.04						5600	10555	25					
11	199.714		594128	606798	294589	310284	645783	589882	519708					
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Insert a new column here.



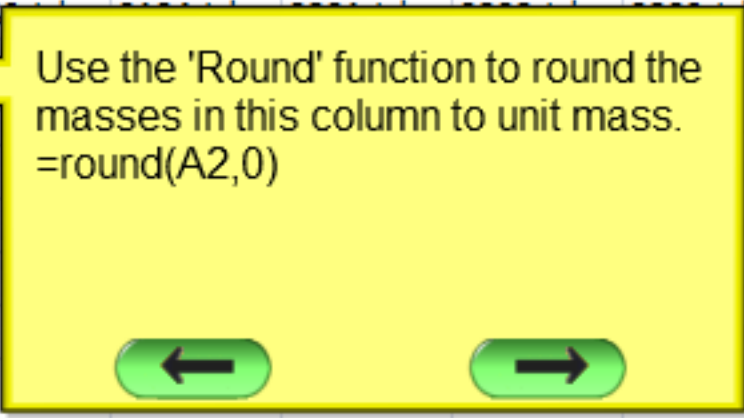
	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	m/z	m/z(nom)	S2S2.tdc					S2S2.tdc	S2S3.tdc					
2	15.036		4					6284	2085					
3	26.994		185					24447	1118					
4	41.029		275					26520	457					
5	27.976		76					12190	81974					
6	42.968		12502	8540	12540	15511	7582	10060	441					
7	73.077		13771	8484	23301	24755	11119	31378	967					
8	104.048		9725	3599	1541	1578	6565	10444	15					
9	148.968		5158	2082	2306	2326	3727	6265	367					
10	104.04		9901	3900	1581	1610	6600	10555	25					
11	199.714		594128	606798	294589	310284	645783	589882	519708					
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Put 'm/z(nom)' in as the column title.



	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	m/z	m/z(nom)	S1S1.tdc	S1S2.tdc	S1S3.tdc	S1S4.tdc	S1S5.tdc	S1S6.tdc	S1S7.tdc	S1S8.tdc	S1S9.tdc	S1S10.tdc	S1S11.tdc	S1S12.tdc
2	15.436	=round(A2,0)												
3	26.994	ROUND(number, num_digits)		22636										
4	41.029		27553	30807										
5	27.976		7693	9782										
6	42.968		12902	8940										
7	73.077		13771	8484										
8	104.048		9725	3599										
9	148.968		5158	2082	2306	2326	3727	6265	367					
10	104.04		9901	3900	1581	1610	6600	10555	25					
11	199.714		594128	606798	294589	310284	645783	589882	519708					
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Use the 'Round' function to round the masses in this column to unit mass.
=round(A2,0)



B2 fx =ROUND(A2,0)

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	m/z	m/z(nom)	S1S1.tdc	S1S2.tdc	S1S3.tdc	S1S4.tdc	S2S1.tdc	S2S2.tdc	S2S3.tdc					
2	15.036	15	4716	5682	1767	1851	5896	6284	2085					
3	26.994	27	18578	22656	4101	4367	26879	24447	1118					
4	41.029	41	27553	30807	1924	1996	37265	26520	457					
5	27.976	28	769					12190	81974					
6	42.968	43						10060	441					
7	73.077	73	1377					31378	967					
8	104.048	104	972					10444	15					
9	148.968	149	515					6265	367					
10	104.04	104	990					10555	25					
11	199.714	200	59412					589882	519708					
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Copy this formula down for all masses.

← →

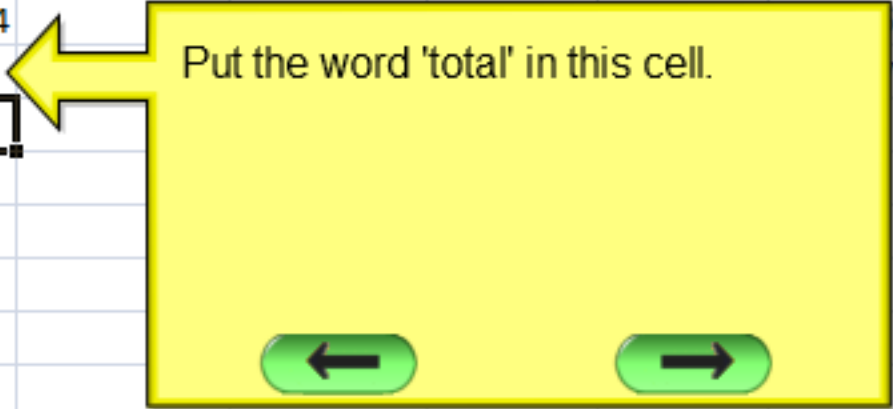
	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	m/z	m/z(nom)	S1S1.tdc	S1S2.tdc	S1S3.tdc	S1S4.tdc	S2S1.tdc	S2S2.tdc	S2S3.tdc					
2	15.036	15	4716	5682	1767	1851	5896	6284	2085					
3	26.994	27	18578	22656	4101	4367	26879	24447	1118					
4	41.029	41	27553	30807	1924	1996	37265	26520	457					
5	27.976	28	7693	9782	34842	40051	6283	12190	81974					
6	42.968	43	12902	8940	12346	13311	7582	10060	441					
7	73.077	73	13771	8484	23301	24755	11119	31378	967					
8	104.048	104	9725	3599	1541	1578	6565	10444	15					
9	148.968	149	5158	2082	2306	2326	3727	6265	367					
10	104.04	104					6600	10555	25					
11	spectrum						645783	589882	519708					
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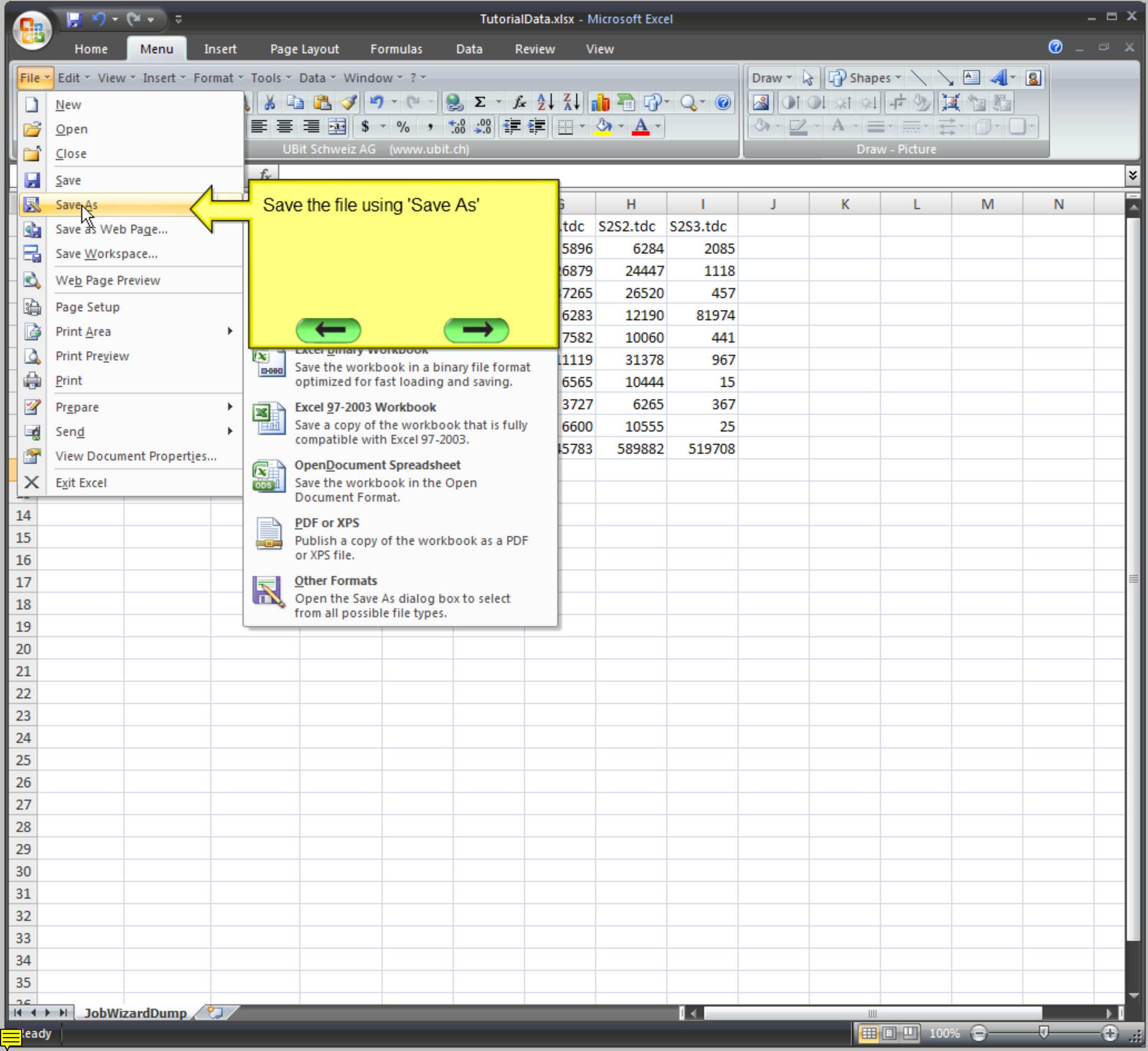
Type 'Spectrum' in this cell. The mass originally shown here is not a real peak. It is a place holder for the total counts for each spectrum.

← →

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	m/z	m/z(nom)	S1S1.tdc	S1S2.tdc	S1S3.tdc	S1S4.tdc	S2S1.tdc	S2S2.tdc	S2S3.tdc					
2	15.036	15	4716	5682	1767	1851	5896	6284	2085					
3	26.994	27	18578	22656	4101	4367	26879	24447	1118					
4	41.029	41	27553	30807	1924	1996	37265	26520	457					
5	27.976	28	7693	9782	34842	40051	6283	12190	81974					
6	42.968	43	12902	8940	12346	13311	7582	10060	441					
7	73.077	73	13771	8484	23301	24755	11119	31378	967					
8	104.048	104	9725	3599	1541	1578	6565	10444	15					
9	148.968	149	5158	2082	2306	2326	3727	6265	367					
10	104.04	104					00	10555	25					
11	spectrum	total					83	589882	519708					
12														
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Put the word 'total' in this cell.





Save the file using 'Save As'



- Excel Binary Workbook**
Save the workbook in a binary file format optimized for fast loading and saving.
- Excel 97-2003 Workbook**
Save a copy of the workbook that is fully compatible with Excel 97-2003.
- OpenDocument Spreadsheet**
Save the workbook in the Open Document Format.
- PDF or XPS**
Publish a copy of the workbook as a PDF or XPS file.
- Other Formats**
Open the Save As dialog box to select from all possible file types.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	m/z	m/z(nom)	S1S1.tdc	S1S2.tdc	S1S3.tdc	S1S4.tdc	S2S1.tdc	S2S2.tdc	S2S3.tdc					
2	15.036	15	4716	5682	1767	1851	5896	6284	2085					
3	26.994	27	18578	22656	4101	4367	26879	24447	1118					
4	41.029													
5	27.976													
6	42.968													
7	73.077													
8	104.048													
9	148.968													
10	104.04													
11	spectrum	total												
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Save As

Save in: PHIData

- watsonfiles
- ~\$TutorialData.xlsx
- Spectra_PeakAreaTable.xlsx
- TutorialData.xlsx

File name: TutorialData.xlsx

Save as type: Excel Workbook (*.xlsx)

- Excel Macro-Enabled Template (*.xltn)
- Excel 97-2003 Template (*.xlt)
- Text (Tab delimited) (*.txt)**
- Unicode Text (*.txt)
- XML Spreadsheet 2003 (*.xml)
- Microsoft Excel 5.0/95 Workbook (*.xls)

Tools

Cancel

Make the 'Save as Type' be 'Text (Tab delimited)(*.txt)

← →

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	m/z	m/z(nom)	S1S1.tdc	S1S2.tdc	S1S3.tdc	S1S4.tdc	S2S1.tdc	S2S2.tdc	S2S3.tdc					
2	15.036	15	4716	5682	1767	1851	5896	6284	2085					
3	26.994	27	18578	22656	4101	4367	26879	24447	1118					
4	41.029													
5	27.976													
6	42.968													
7	73.077													
8	104.048													
9	148.968													
10	104.04													
11	spectrum	total												
12														
13														
14														
15														
16														
17														
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32														
33														
34														
35														

Save As

Save in: PHIData

- watsonfiles
- phitesttable.txt

My Recent Documents

Desktop

My Documents

My Computer

My Network Places

File name: TutorialData.txt

Save as type: Text (Tab delimited) (*.txt)

Tools

Save Cancel

Give the file a name.

← →

	A	B	C	D	E	F	G	H	I
1	m/z	m/z(nom)	S1S1.tdc	S1S2.tdc	S1S3.tdc	S1S4.tdc	S2S1.tdc	S2S2.tdc	S2S3.tdc
2	15.036	15	4716	5682	1767	1851	5896	6284	2085
3	26.994	27	18578	22656	4101	4367	26879	24447	1118
4	41.029								
5	27.976								
6	42.968								
7	73.077								
8	104.048								
9	148.968								
10	104.04								
11	spectrum	total							
12									

Because it is required for the import script it is a good idea to note the number of spectra in the file in the filename. Here there are 7 files.

← →

Save As

Save in: PHIData

- watsonfiles
- phitesttable.txt

My Recent Documents

Desktop

My Documents

My Computer

My Network Places

File name: TutorialData.txt

Save as type: Text (Tab delimited) (*.txt)

Tools Save Cancel

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	m/z	m/z(nom)	S1S1.tdc	S1S2.tdc	S1S3.tdc	S1S4.tdc	S2S1.tdc	S2S2.tdc	S2S3.tdc					
2	15.036	15	4716	5682	1767	1851	5896	6284	2085					
3	26.994	27	18578	22656	4101	4367	26879	24447	1118					
4	41.029													
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8	104.048													
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10	104.04													
11	spectrum	total												
12														
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33														
34														
35														

Save As

Save in: PHIData

- watsonfiles
- phitesttable.txt

My Recent Documents

Desktop

My Documents

My Computer

My Network Places

File name: TutorialData7.txt

Save as type: Text (Tab delimited) (*.txt)

Tools

Save Cancel

So I will add a 7 to the filename. Remember you must know the number of spectra in your file for the import script to work.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	m/z	m/z(nom)	S1S1.tdc	S1S2.tdc	S1S3.tdc	S1S4.tdc	S2S1.tdc	S2S2.tdc	S2S3.tdc					
2	15.036	15	4716	5682	1767	1851	5896	6284	2085					
3	26.994	27	18578	22656	4101	4367	26879	24447	1118					
4	41.029													
5	27.976													
6	42.968													
7	73.077													
8	104.048													
9	148.968													
10	104.04													
11	spectrum	total												
12														

Save As

Save in: PHIData

- watsonfiles
- phitesttable.txt

My Recent Documents

Desktop

My Documents

My Computer

My Network Places

File name: TutorialData7.txt

Save as type: Text (Tab delimited) (*.txt)

Tools

Save Cancel

Make sure the file is being saved in your active matlab folder.

Press the 'Save' button to save the file.

← →

TutorialData7.txt Microsoft Excel

Home Menu Insert Page Layout Formulas Data Review View

File Edit View Insert Format Tools Data Window ?

Calibri 11 B I U \$ % .00 .00

Ubit Schweiz AG (www.ubit.ch)

Draw Shapes

Draw - Picture

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	m/z	m/z(nom)	S1S1.tdc	S1S2.tdc	S1S3.tdc	S1S4.tdc	S2S1.tdc	S2S2.tdc	S2S3.tdc					
2	15.036	15	4716	5682	1767	1851	5896	6284	2085					
3	26.994	27	18578	22656	4101	4367	26879	24447	1118					
4	41.029	41	27553	30807	1924	1996	37265	26520	457					
5	27.976	28	7693	9782	34842	40051	6283	12190	81974					
6	42.968	43	12902	8940	12346	13311	7582	10060	441					
7	73.077	73	13771	8484	23301	24755	11119	31378	967					
8	104.048	104	9725	3599	1541	1578	6565	10444	15					
9	148.968	149	5158	2082	2306	2326	3727	6265	367					
10	104.04	104	9901	3900	1581	1610	6600	10555	25					
11	spectrum	total	594128	606798	294589	310284	645783	589882	519708					
12														

Microsoft Office Excel

TutorialData7.txt may contain features that are not compatible with Text (Tab delimited). Do you want to keep the workbook in this format?

- To keep this format, which leaves out any incompatible features, click Yes.
- To preserve the features, click No. Then save a copy in the latest Excel format.
- To see what might be lost, click Help.

Yes

Press 'Yes' to keep the current format.

← →

spectragui

File Data Pre-Processing MVA Data Display extra

- Import Data
 - Physical Electronics
 - IonTof
 - Import from Workspace
- Create Sample Names
- Normalize Data
- Delete Samples
- Delete Variables (Peaks)
- Sub Divide Matrix

These are the main input data
Use the drop down menus to s

Name of Variable Matrix

Select Data Select Variables

alcounts Matrix Name of Samplenames Matrix

alcounts Select Samples

Within the spectragui from the 'Data Pre-Processing' menu choose -> Import Data -> Physical Electronics

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
---	--	--	---	---

PHI Data import (Tofpak Output)

Name of .txt. file

tutorialdata7.txt

Number of Files in Data Set

7

Import Data

Close Panel

Enter the full name of the file including the .txt extension.

Enter the number of files(spectra) in the data set and press the 'Import Data' button.



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

Select Data

data

Name of Variable Matrix

Select Variables

Name of Filename Matrix

Select Filenames

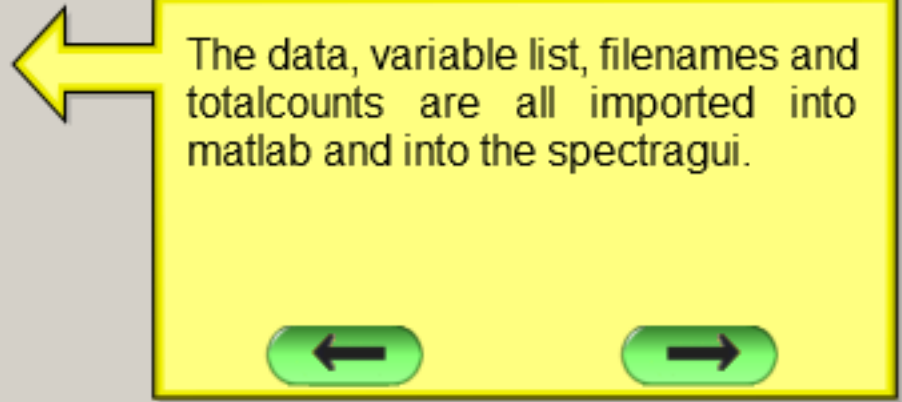
Name of Totalcounts Matrix

Select Totalcounts

Name of Samplenames Matrix

Select Samples

The data, variable list, filenames and totalcounts are all imported into matlab and into the spectragui.



Workspace

Name	Value
data	<7x9 double>
exactmass	<9x8 char>
filenames	<7x8 char>
nommass	<9x8 char>
totalcounts	[594128;606796]

Command Window

```
>> spectragui
>> filenames

filenames =

S1S1.tdc
S1S2.tdc
S1S3.tdc
S1S4.tdc
S2S1.tdc
S2S2.tdc
S2S3.tdc

>> |
```

Here we show the filenames imported. As expected they match the names in the file we imported.

Workspace

Name	Value
data	<7x9 double>
exactmass	<9x8 char>
filenames	<7x8 char>
nommass	<9x8 char>
totalcounts	[594128;606796]

Command Window

```
>> spectragui  
>> filenames
```

```
filenames =
```

```
S1S1.tdc
```

```
S1S2.tdc
```

```
S1S3.tdc
```

```
S1S4.tdc
```

```
S2S1.tdc
```

```
S2S2.tdc
```

```
S2S3.tdc
```

```
>>
```

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.

