

### Data Selection Panel

These are the main input data that will be used in further analysis unless you specify otherwise. Use the drop down menus to select the data and information you want to use in your analysis.

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

This tutorial contains navigation buttons that enable you to move throughout the tutorial.

Please use the navigation buttons and not the page up/page down or arrow keys to navigate through the tutorials.

This is the 'Next' button. It takes you to the next frame or stop point.



This is the 'Previous' button. It takes you to the previous frame or stop point.



This is the 'Go to frame' button. It takes you to a specified frame.



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



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






Workspace


Name

Command Window

```
>>  
>> |
```

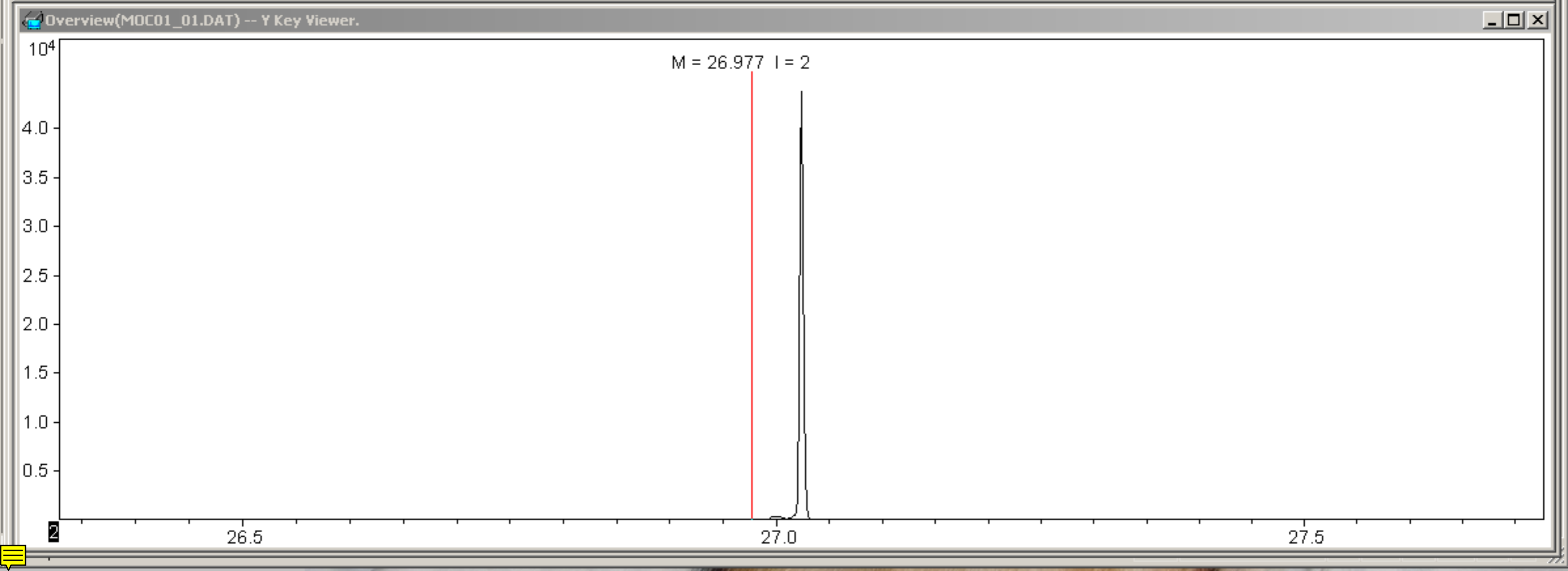
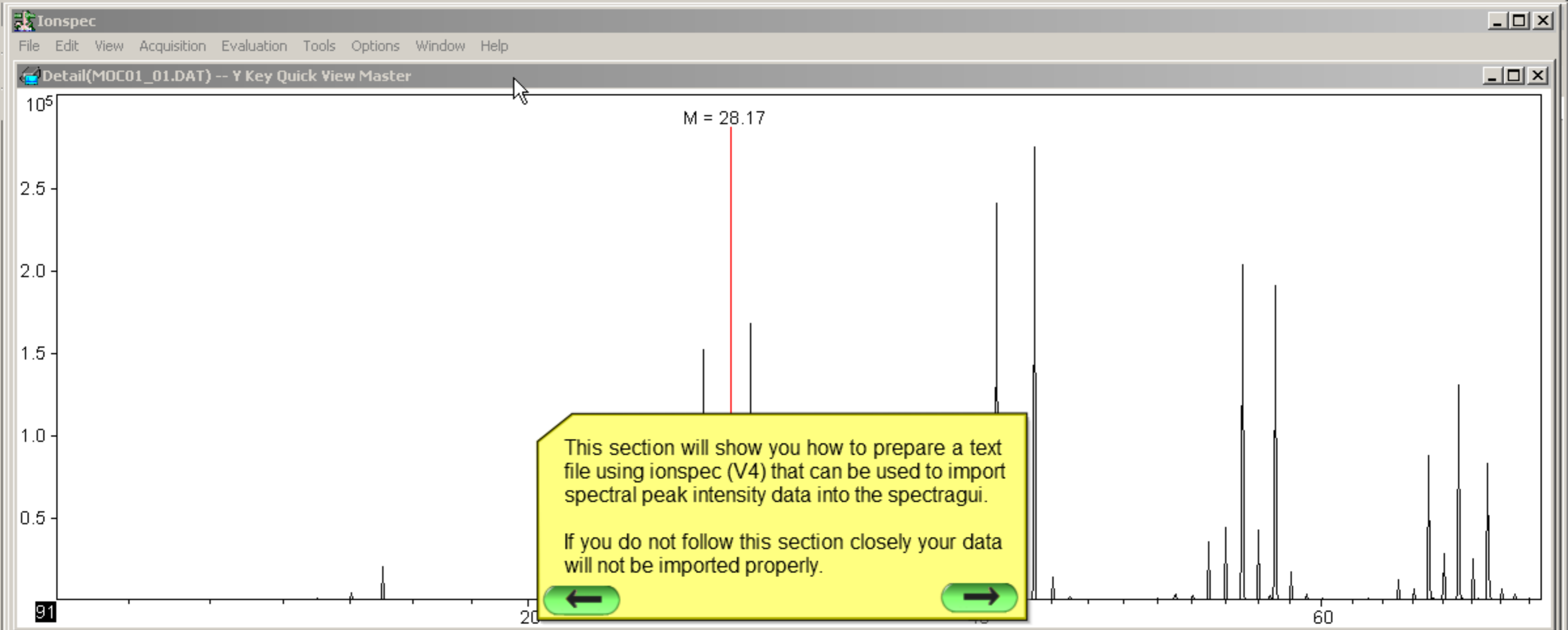
This tutorial will cover loading an iontof data

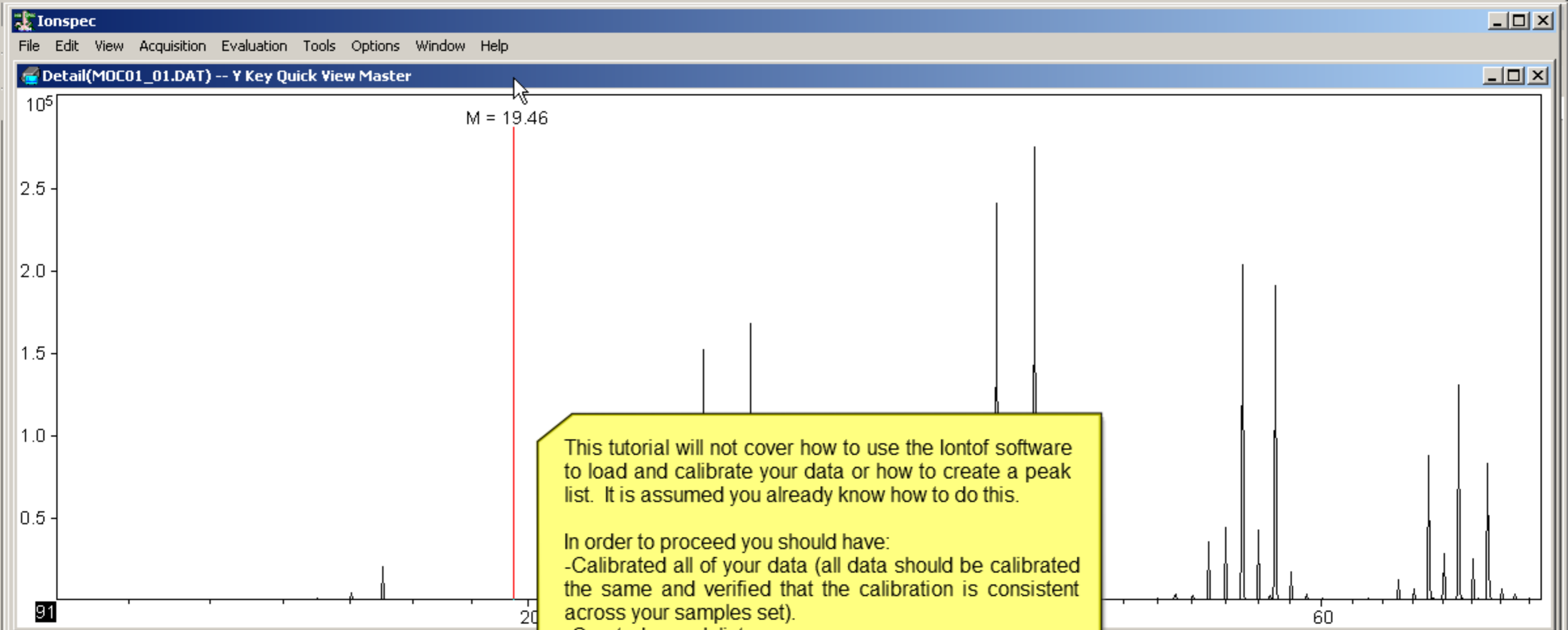
Press this button if you are using the lonspec (V4)	Press this button if you are using Measurement explorer (spectra) (V6)	Press this button to learn about importing .xlsx files
		



Command History

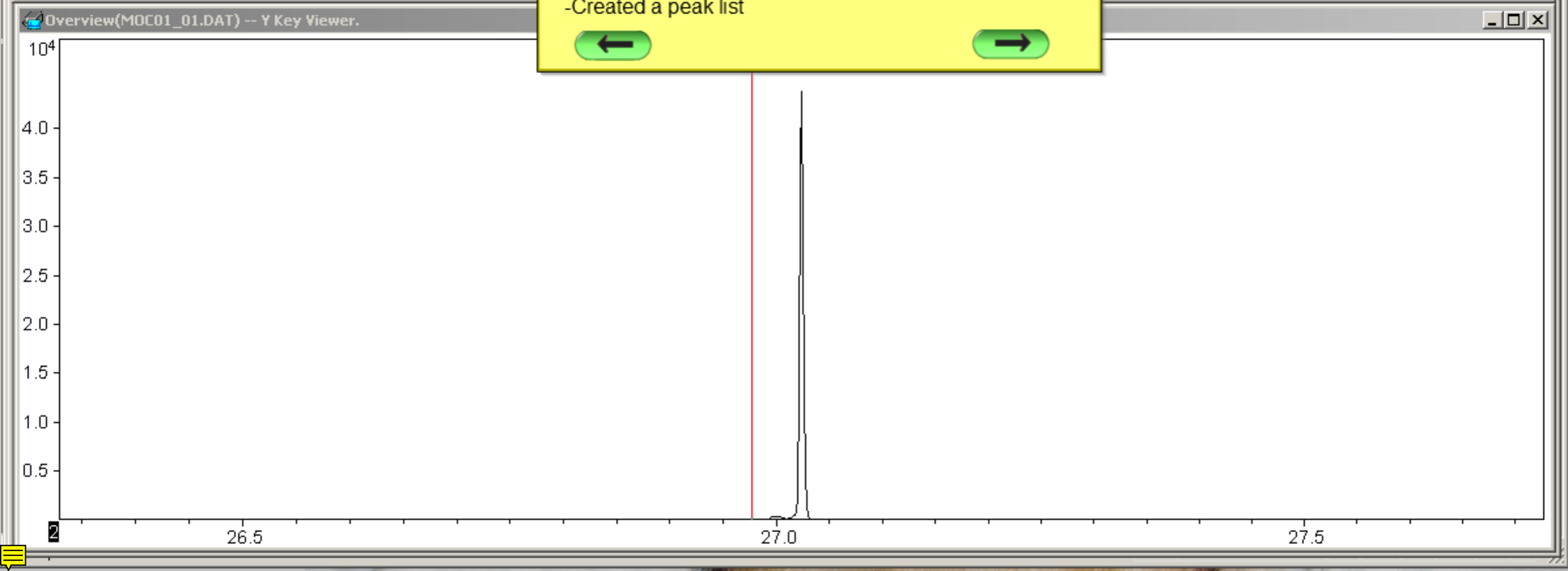
```
---%-- 8/13/10 9:4
```

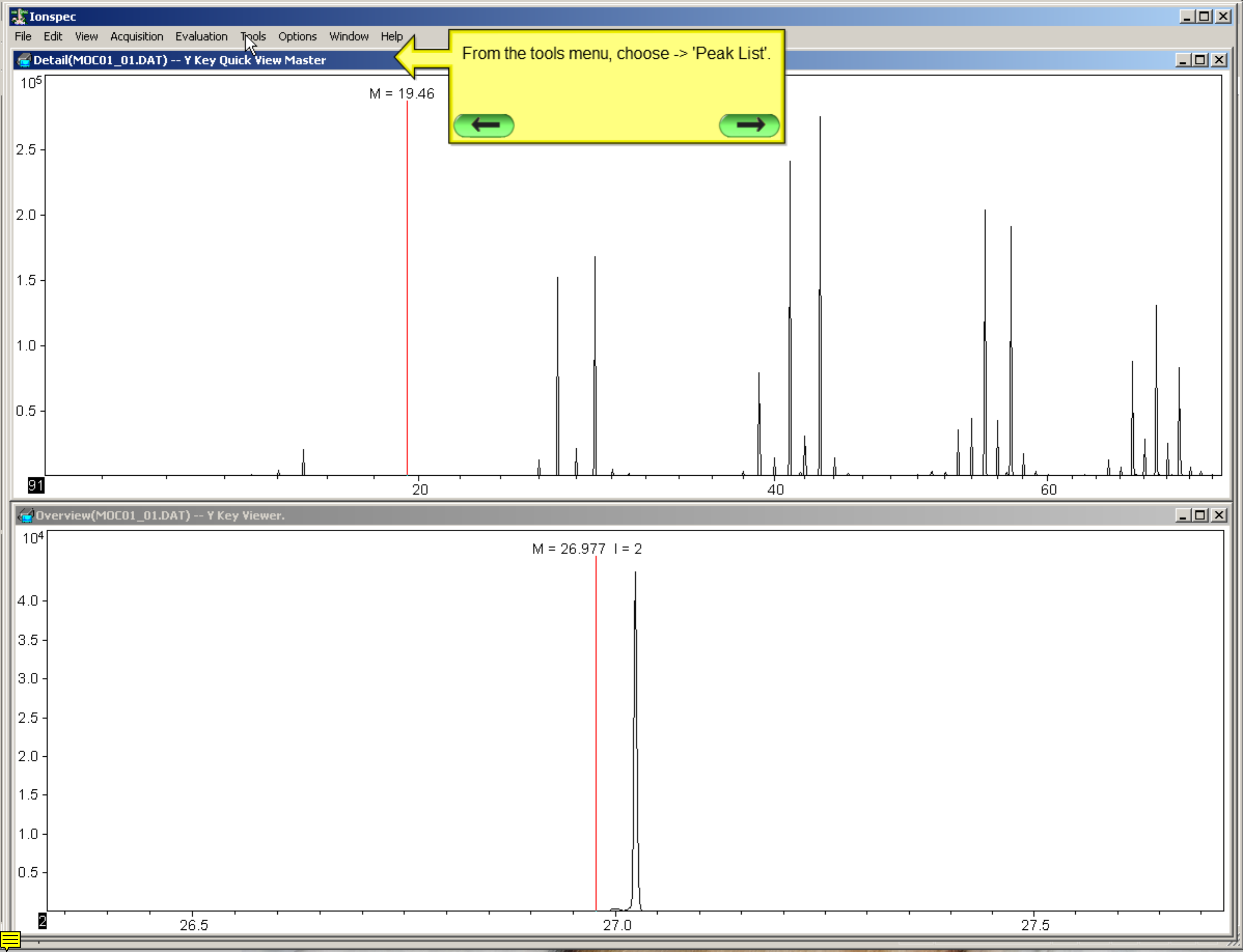


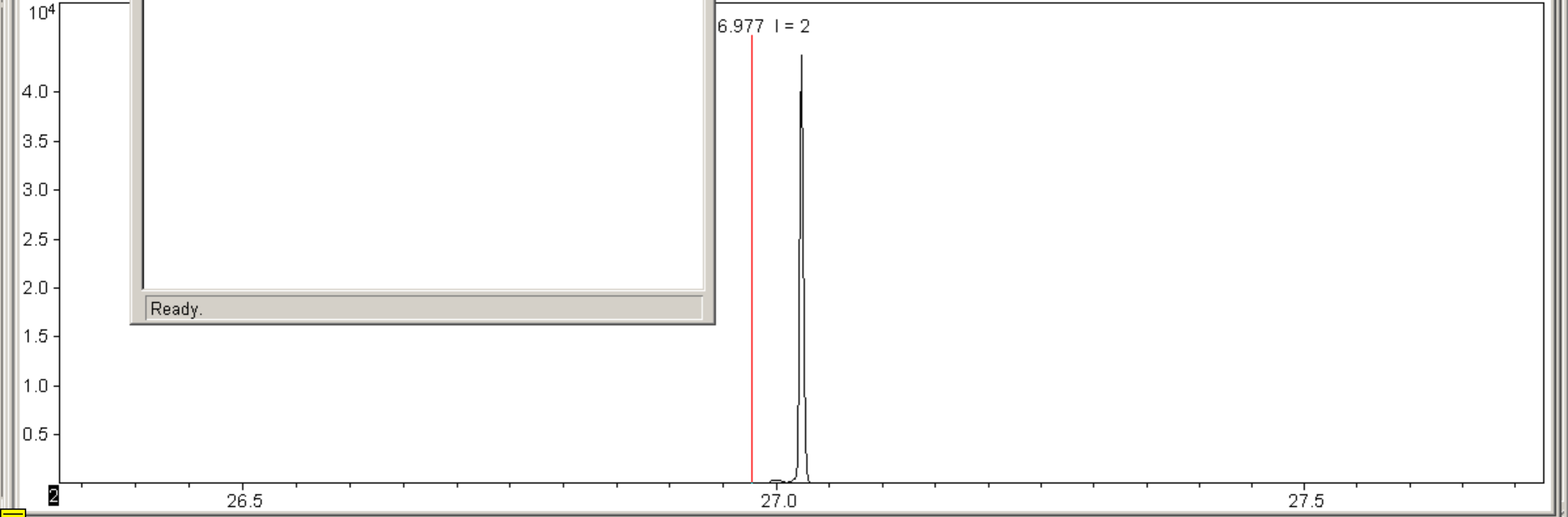
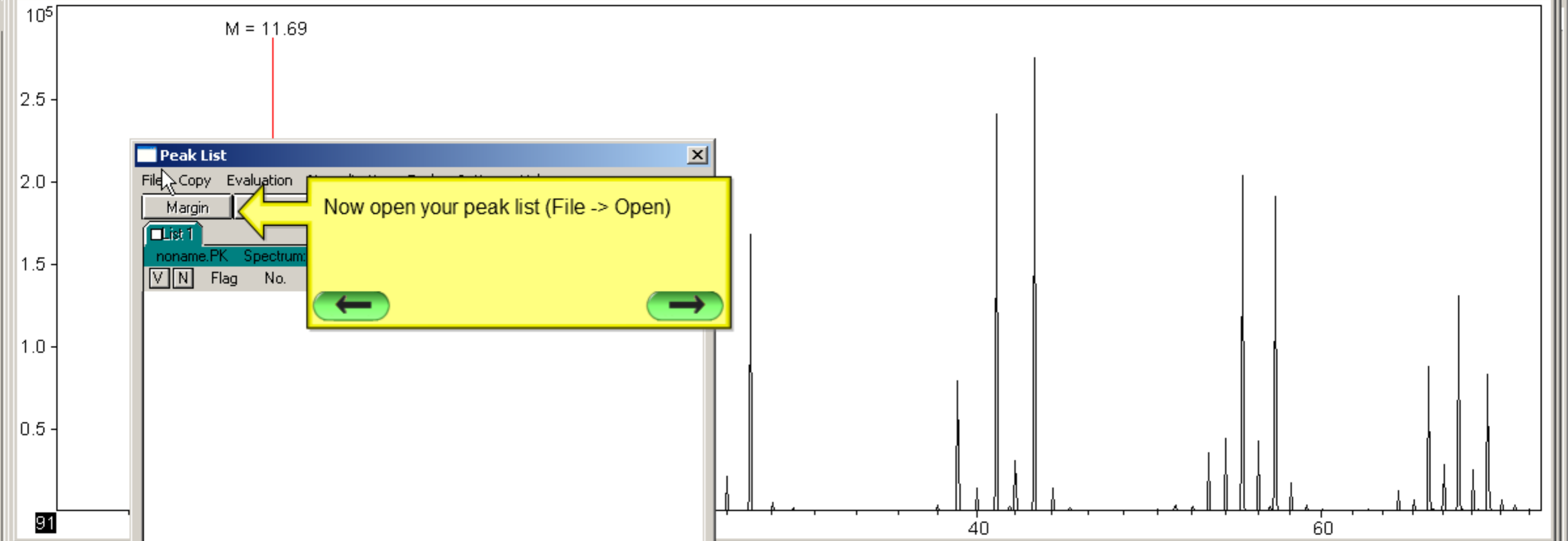


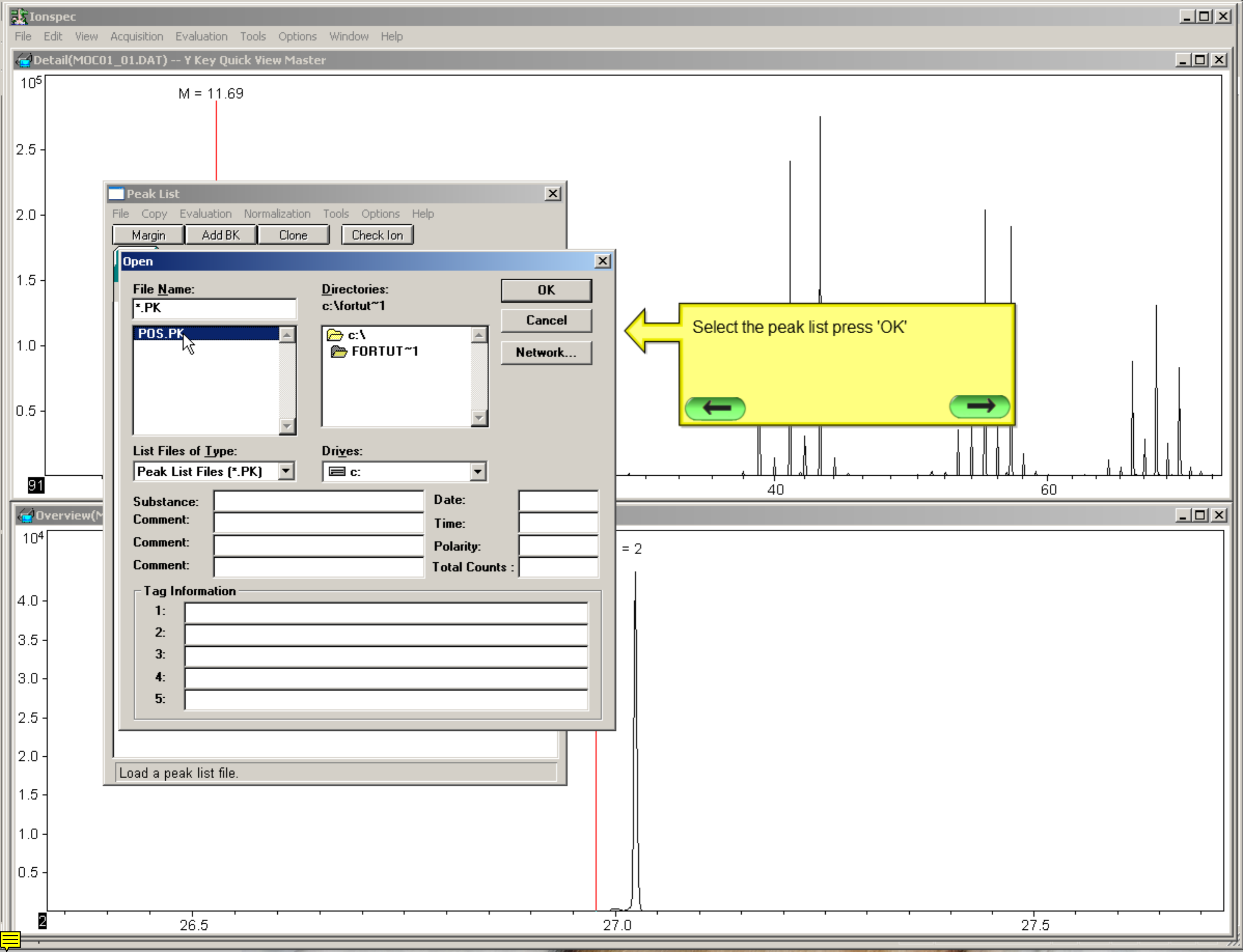
This tutorial will not cover how to use the Iontof software to load and calibrate your data or how to create a peak list. It is assumed you already know how to do this.

- In order to proceed you should have:
- Calibrated all of your data (all data should be calibrated the same and verified that the calibration is consistent across your samples set).
  - Created a peak list









M = 11.69

Peak List

File Copy Evaluation Normalization Tools Options Help

Margin Add BK Clone Check Ion

Open

File Name:

\*.PK

Directories:

c:\fortut~1

OK

Cancel

Network...

- POS.PK

List Files of Type:

Peak List Files (\*.PK)

Drives:

c:

Substance:

Date:

Comment:

Time:

Comment:

Polarity:

Comment:

Total Counts:

Tag Information

- 1:
- 2:
- 3:
- 4:
- 5:

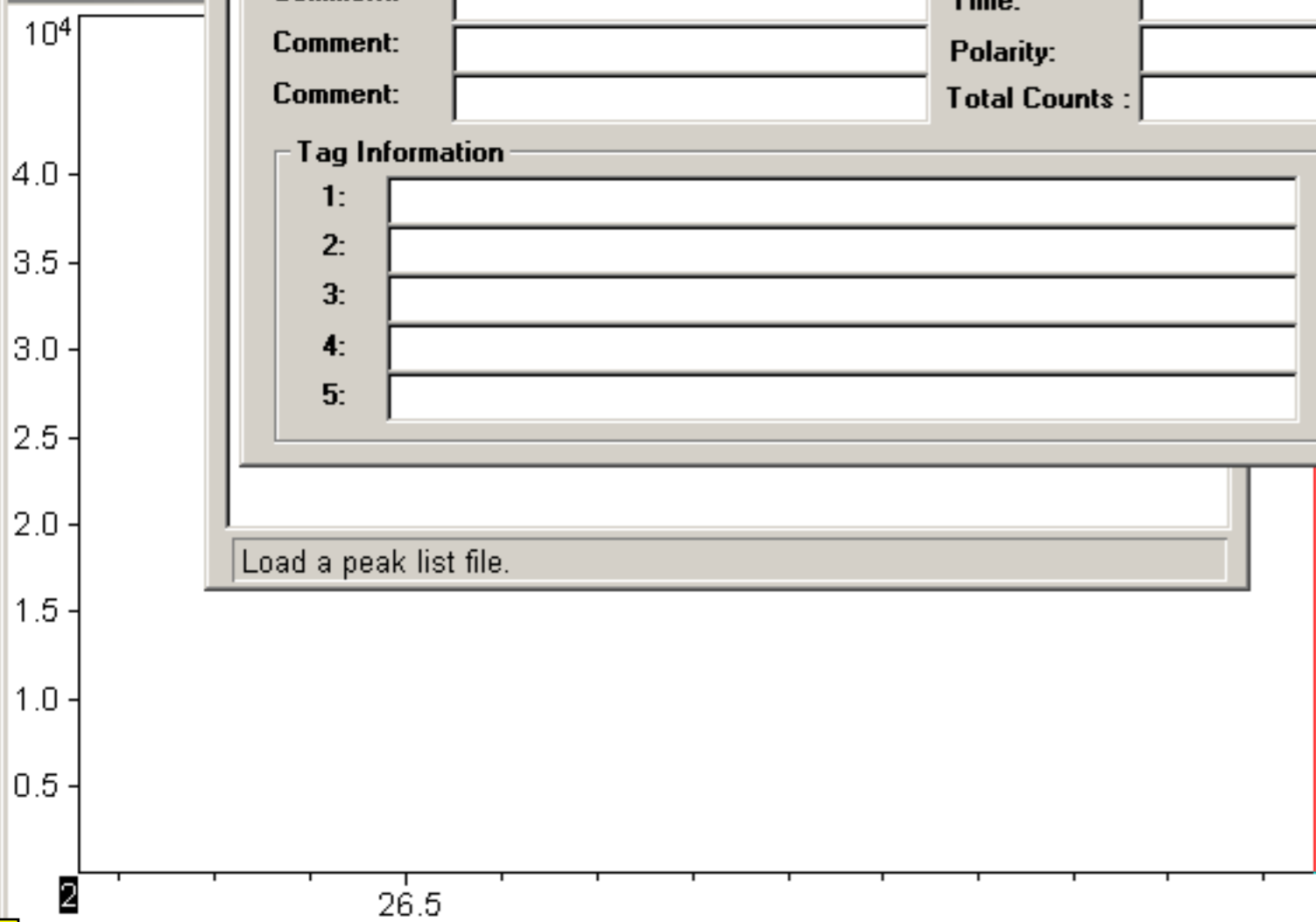
Load a peak list file.

Select the peak list press 'OK'



91

Overview(M

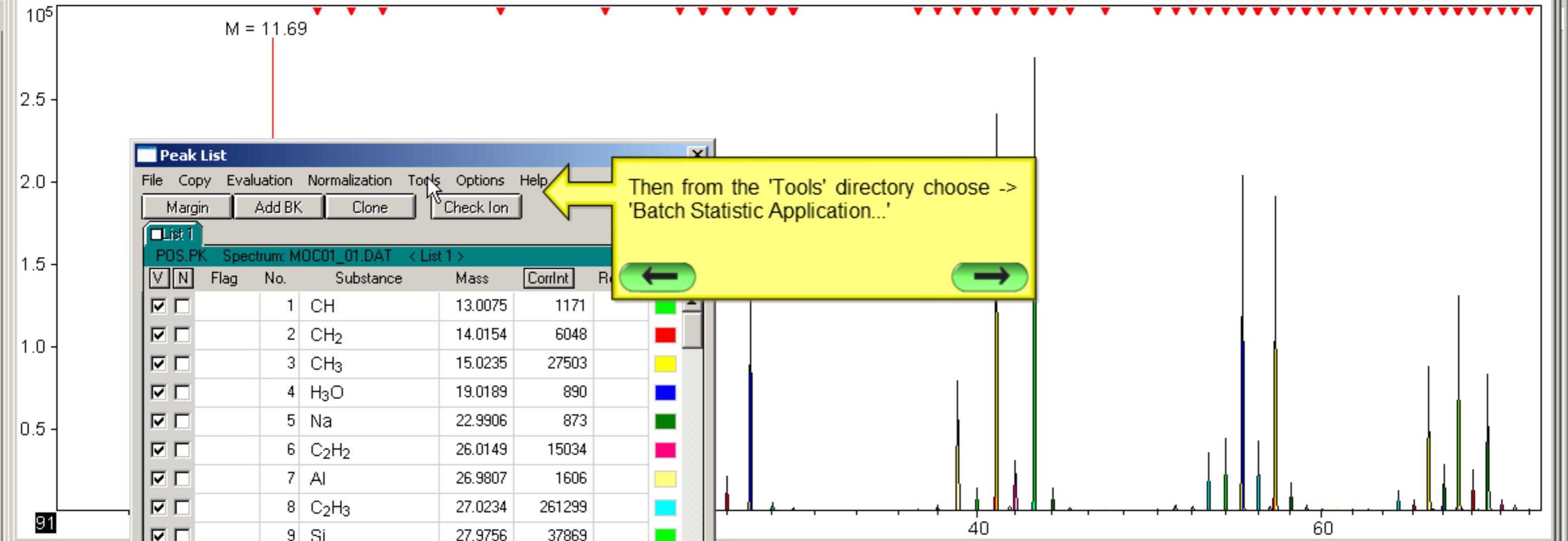


= 2

26.5

27.0

27.5



**Peak List**

File Copy Evaluation Normalization Tools Options Help

Margin Add BK Clone Check Ion

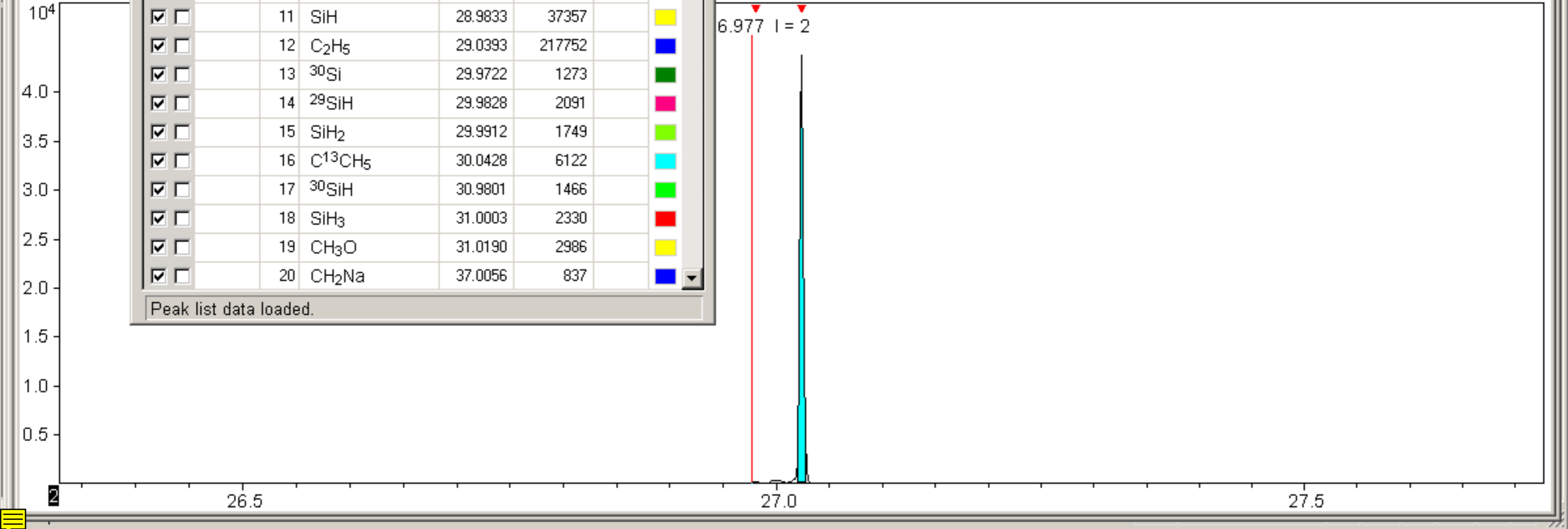
List 1

POS.PK Spectrum: MOC01\_01.DAT < List 1 >

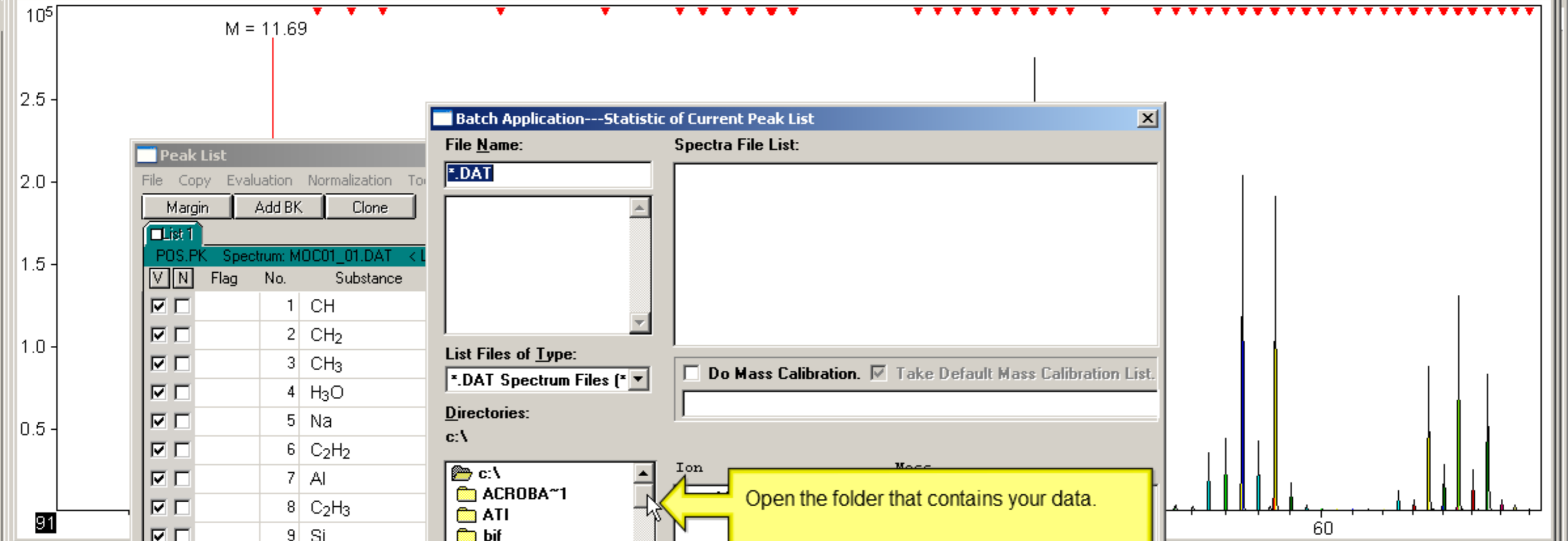
V	N	Flag	No.	Substance	Mass	CorrInt	R
<input checked="" type="checkbox"/>	<input type="checkbox"/>		1	CH	13.0075	1171	
<input checked="" type="checkbox"/>	<input type="checkbox"/>		2	CH <sub>2</sub>	14.0154	6048	
<input checked="" type="checkbox"/>	<input type="checkbox"/>		3	CH <sub>3</sub>	15.0235	27503	
<input checked="" type="checkbox"/>	<input type="checkbox"/>		4	H <sub>3</sub> O	19.0189	890	
<input checked="" type="checkbox"/>	<input type="checkbox"/>		5	Na	22.9906	873	
<input checked="" type="checkbox"/>	<input type="checkbox"/>		6	C <sub>2</sub> H <sub>2</sub>	26.0149	15034	
<input checked="" type="checkbox"/>	<input type="checkbox"/>		7	Al	26.9807	1606	
<input checked="" type="checkbox"/>	<input type="checkbox"/>		8	C <sub>2</sub> H <sub>3</sub>	27.0234	261299	
<input checked="" type="checkbox"/>	<input type="checkbox"/>		9	Si	27.9756	37869	
<input checked="" type="checkbox"/>	<input type="checkbox"/>		10	C <sub>2</sub> H <sub>4</sub>	28.0310	22071	
<input checked="" type="checkbox"/>	<input type="checkbox"/>		11	SiH	28.9833	37357	
<input checked="" type="checkbox"/>	<input type="checkbox"/>		12	C <sub>2</sub> H <sub>5</sub>	29.0393	217752	
<input checked="" type="checkbox"/>	<input type="checkbox"/>		13	<sup>30</sup> Si	29.9722	1273	
<input checked="" type="checkbox"/>	<input type="checkbox"/>		14	<sup>29</sup> SiH	29.9828	2091	
<input checked="" type="checkbox"/>	<input type="checkbox"/>		15	SiH <sub>2</sub>	29.9912	1749	
<input checked="" type="checkbox"/>	<input type="checkbox"/>		16	C <sup>13</sup> CH <sub>5</sub>	30.0428	6122	
<input checked="" type="checkbox"/>	<input type="checkbox"/>		17	<sup>30</sup> SiH	30.9801	1466	
<input checked="" type="checkbox"/>	<input type="checkbox"/>		18	SiH <sub>3</sub>	31.0003	2330	
<input checked="" type="checkbox"/>	<input type="checkbox"/>		19	CH <sub>3</sub> O	31.0190	2986	
<input checked="" type="checkbox"/>	<input type="checkbox"/>		20	CH <sub>2</sub> Na	37.0056	837	

Peak list data loaded.

Then from the 'Tools' directory choose -> 'Batch Statistic Application...'







Peak List

File Copy Evaluation Normalization To

Margin Add BK Clone

List 1

POS.PK Spectrum: MOC01\_01.DAT < 1

V	N	Flag	No.	Substance				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		1	CH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		2	CH <sub>2</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		3	CH <sub>3</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		4	H <sub>3</sub> O				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		5	Na				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		6	C <sub>2</sub> H <sub>2</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		7	Al				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		8	C <sub>2</sub> H <sub>3</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		9	Si				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		10	C <sub>2</sub> H <sub>4</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		11	SiH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		12	C <sub>2</sub> H <sub>5</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		13	<sup>30</sup> Si				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		14	<sup>29</sup> SiH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		15	SiH <sub>2</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		16	C <sup>13</sup> CH <sub>5</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		17	<sup>30</sup> SiH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		18	SiH <sub>3</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		19	CH <sub>3</sub> O	31.0190	2986		Yellow
<input checked="" type="checkbox"/>	<input type="checkbox"/>		20	CH <sub>2</sub> Na	37.0056	837		Blue

Open intensity statistic window.

Batch Application---Statistic of Current Peak List

File Name: \*.DAT

Spectra File List:

List Files of Type: \*.DAT Spectrum Files (\*)

Directories: c:\

- c:\
- ACROBA~1
- ATI
- bif
- cabs
- data
- dell

Drives: c:

Polarity: Positive SIMS

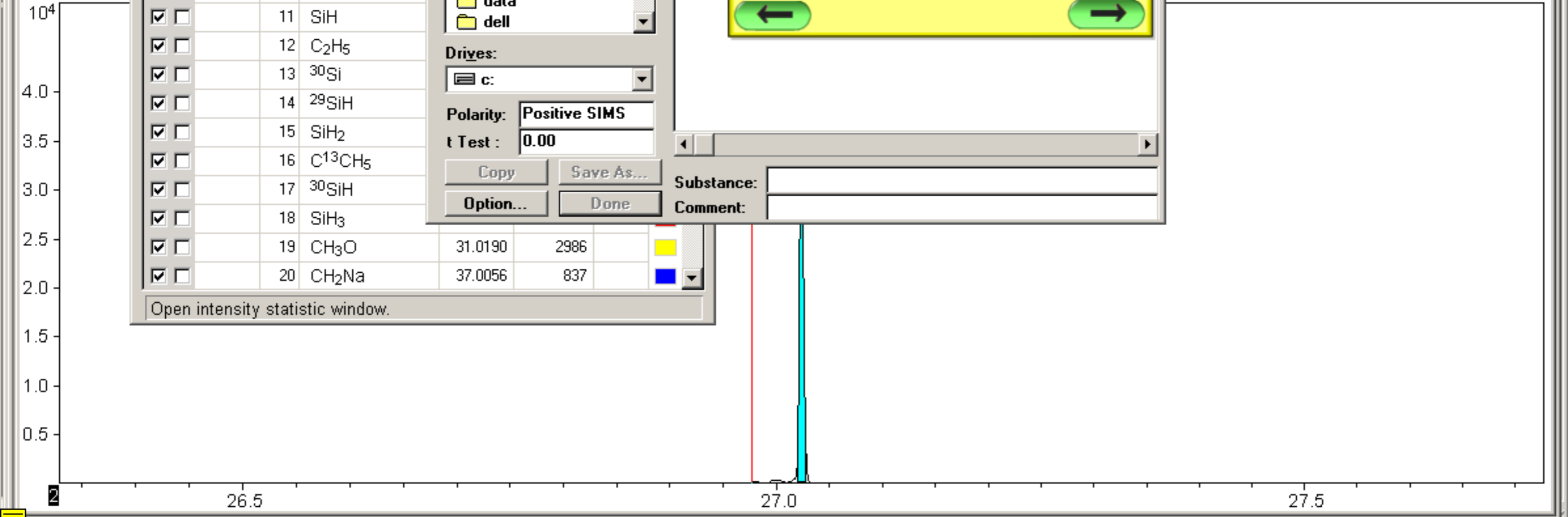
t Test: 0.00

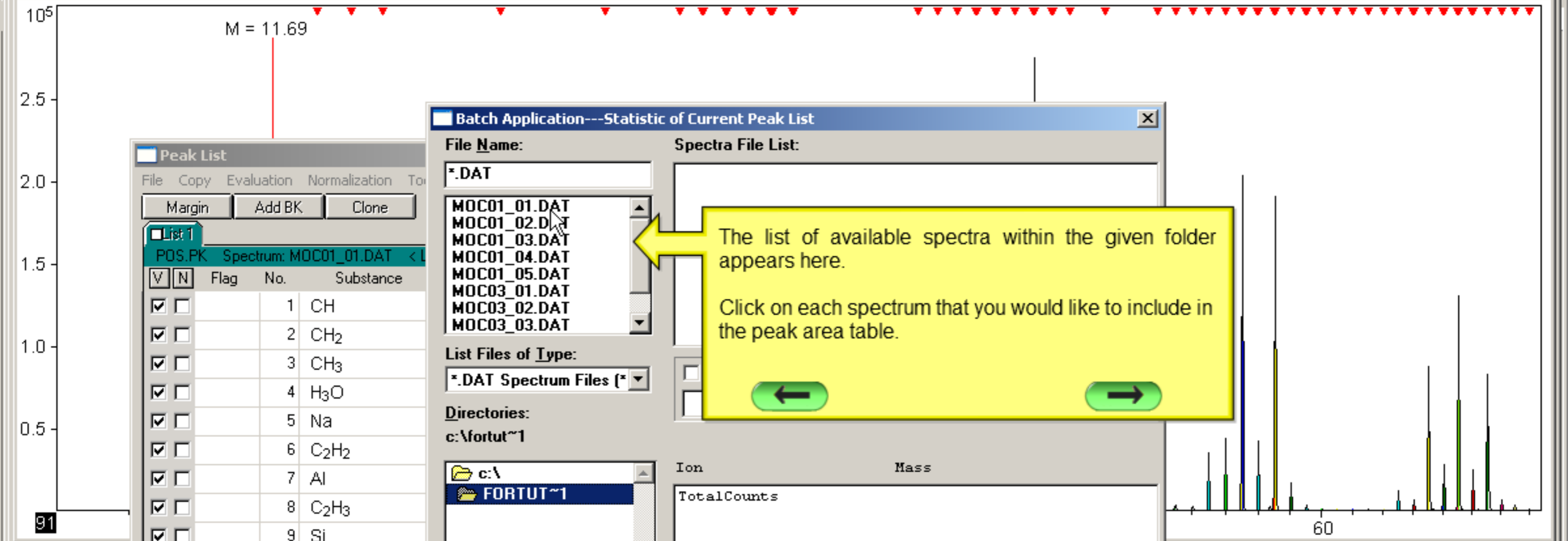
Substance:

Comment:

Copy Save As... Option... Done

Open the folder that contains your data.





Peak List								
File	Copy	Evaluation	Normalization	To				
Margin	Add BK	Clone						
<input type="checkbox"/>	List 1							
POS.PK	Spectrum: MOC01_01.DAT	<						
V	N	Flag	No.	Substance				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		1	CH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		2	CH <sub>2</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		3	CH <sub>3</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		4	H <sub>3</sub> O				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		5	Na				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		6	C <sub>2</sub> H <sub>2</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		7	Al				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		8	C <sub>2</sub> H <sub>3</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		9	Si				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		10	C <sub>2</sub> H <sub>4</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		11	SiH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		12	C <sub>2</sub> H <sub>5</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		13	<sup>30</sup> Si				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		14	<sup>29</sup> SiH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		15	SiH <sub>2</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		16	C <sup>13</sup> CH <sub>5</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		17	<sup>30</sup> SiH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		18	SiH <sub>3</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		19	CH <sub>3</sub> O	31.0190	2986		Yellow
<input checked="" type="checkbox"/>	<input type="checkbox"/>		20	CH <sub>2</sub> Na	37.0056	837		Blue

**Batch Application---Statistic of Current Peak List**

File Name: \*.DAT

Spectra File List:

- MOC01\_01.DAT
- MOC01\_02.DAT
- MOC01\_03.DAT
- MOC01\_04.DAT
- MOC01\_05.DAT
- MOC03\_01.DAT
- MOC03\_02.DAT
- MOC03\_03.DAT

List Files of Type: \*.DAT Spectrum Files (\*)

Directories: c:\fortut~1

Drives: c:

Polarity: Positive SIMS

t Test: 0.00

Copy Save As... Option... Done

Substance: \_\_\_\_\_

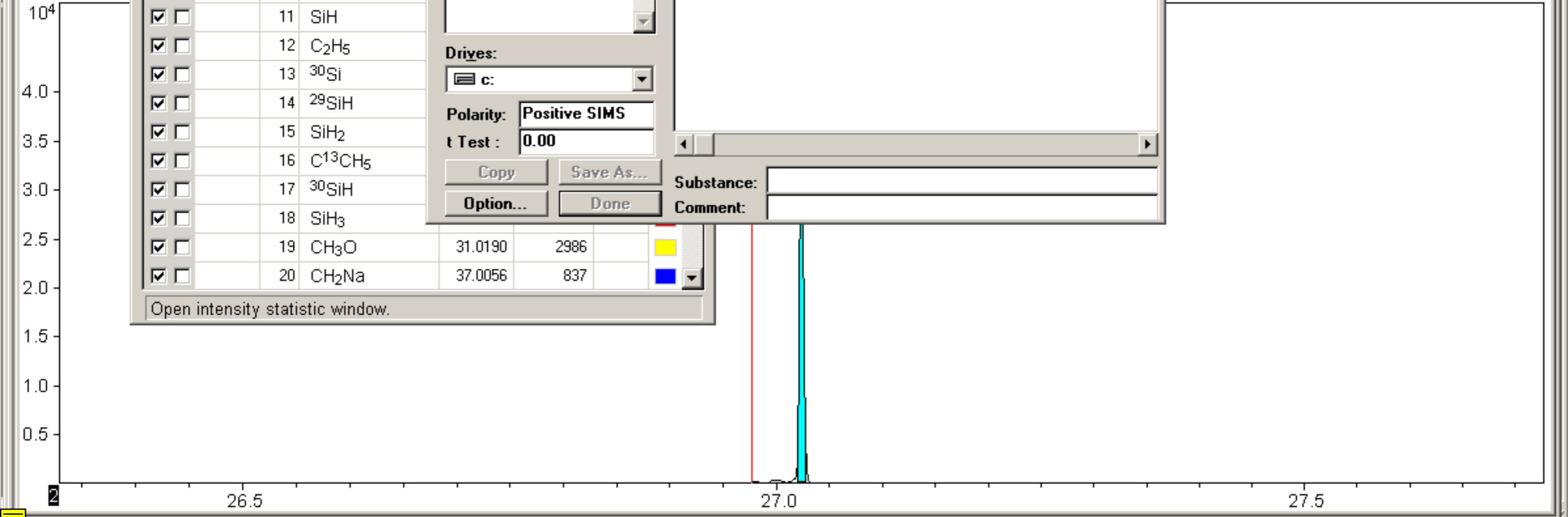
Comment: \_\_\_\_\_

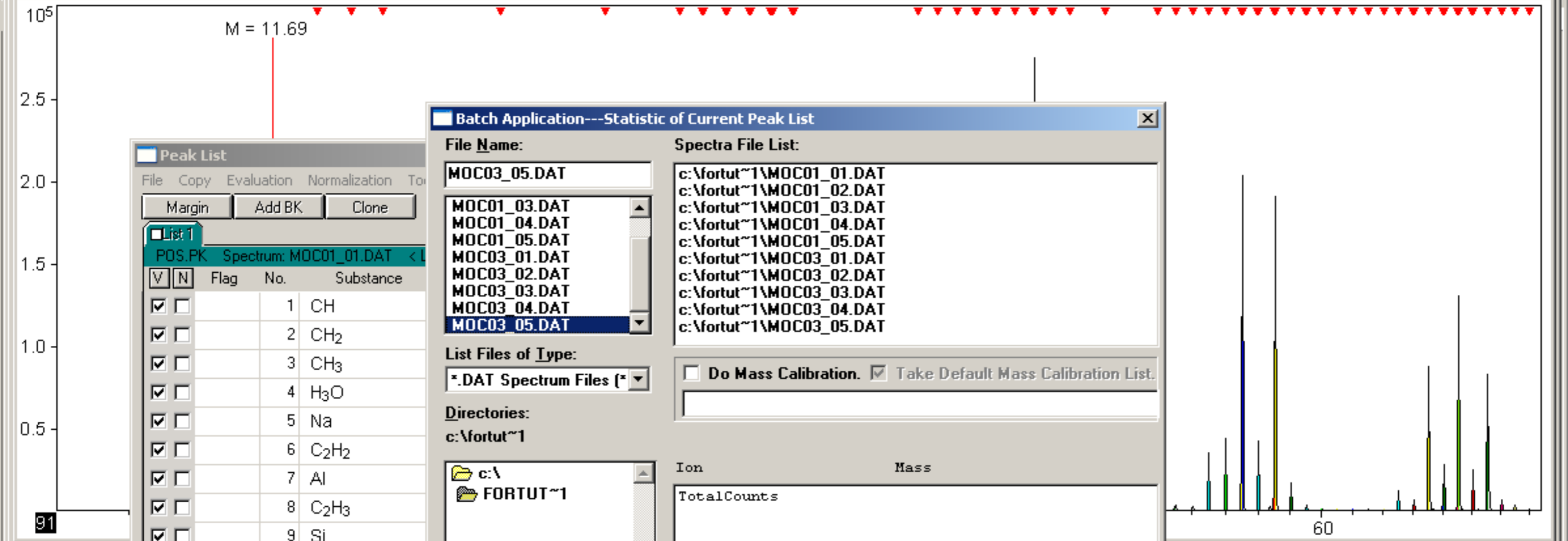
Ion Mass

TotalCounts

The list of available spectra within the given folder appears here.

Click on each spectrum that you would like to include in the peak area table.





Peak List

File Copy Evaluation Normalization To

Margin Add BK Clone

List 1

POS.PK Spectrum: MOC01\_01.DAT <1

V	N	Flag	No.	Substance
<input checked="" type="checkbox"/>	<input type="checkbox"/>		1	CH
<input checked="" type="checkbox"/>	<input type="checkbox"/>		2	CH <sub>2</sub>
<input checked="" type="checkbox"/>	<input type="checkbox"/>		3	CH <sub>3</sub>
<input checked="" type="checkbox"/>	<input type="checkbox"/>		4	H <sub>3</sub> O
<input checked="" type="checkbox"/>	<input type="checkbox"/>		5	Na
<input checked="" type="checkbox"/>	<input type="checkbox"/>		6	C <sub>2</sub> H <sub>2</sub>
<input checked="" type="checkbox"/>	<input type="checkbox"/>		7	Al
<input checked="" type="checkbox"/>	<input type="checkbox"/>		8	C <sub>2</sub> H <sub>3</sub>
<input checked="" type="checkbox"/>	<input type="checkbox"/>		9	Si
<input checked="" type="checkbox"/>	<input type="checkbox"/>		10	C <sub>2</sub> H <sub>4</sub>

Batch Application---Statistic of Current Peak List

File Name: MOC03\_05.DAT

Spectra File List:

- c:\fortut~1\MOC01\_01.DAT
- c:\fortut~1\MOC01\_02.DAT
- c:\fortut~1\MOC01\_03.DAT
- c:\fortut~1\MOC01\_04.DAT
- c:\fortut~1\MOC01\_05.DAT
- c:\fortut~1\MOC03\_01.DAT
- c:\fortut~1\MOC03\_02.DAT
- c:\fortut~1\MOC03\_03.DAT
- c:\fortut~1\MOC03\_04.DAT
- c:\fortut~1\MOC03\_05.DAT

List Files of Type: \*.DAT Spectrum Files (\*)

Directories: c:\fortut~1

Ion Mass

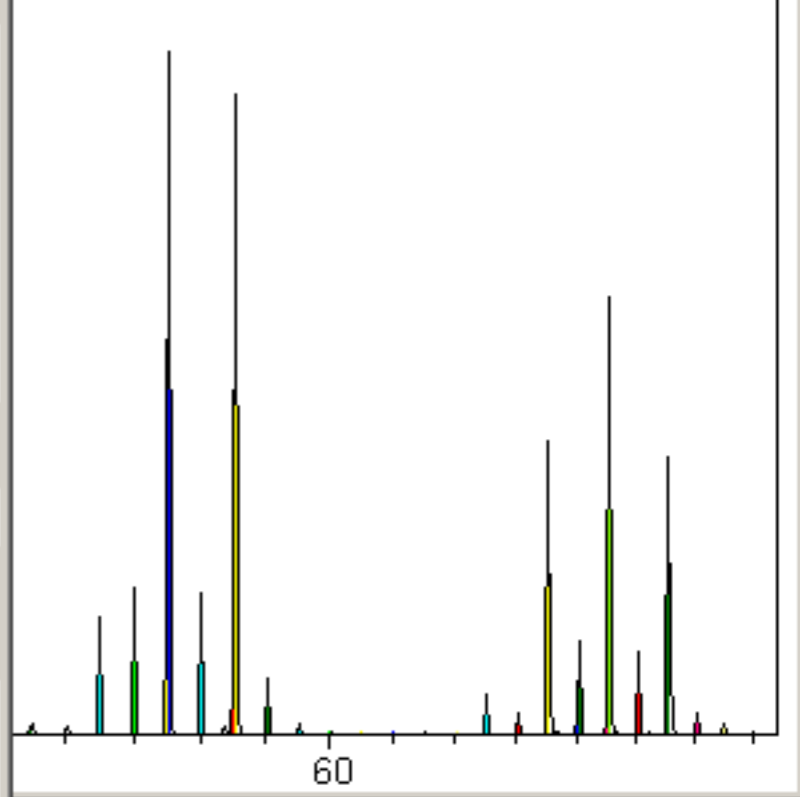
Ion	Mass
TotalCounts	

Do Mass Calibration.  Take Default Mass Calibration List.

Substance:

Comment:

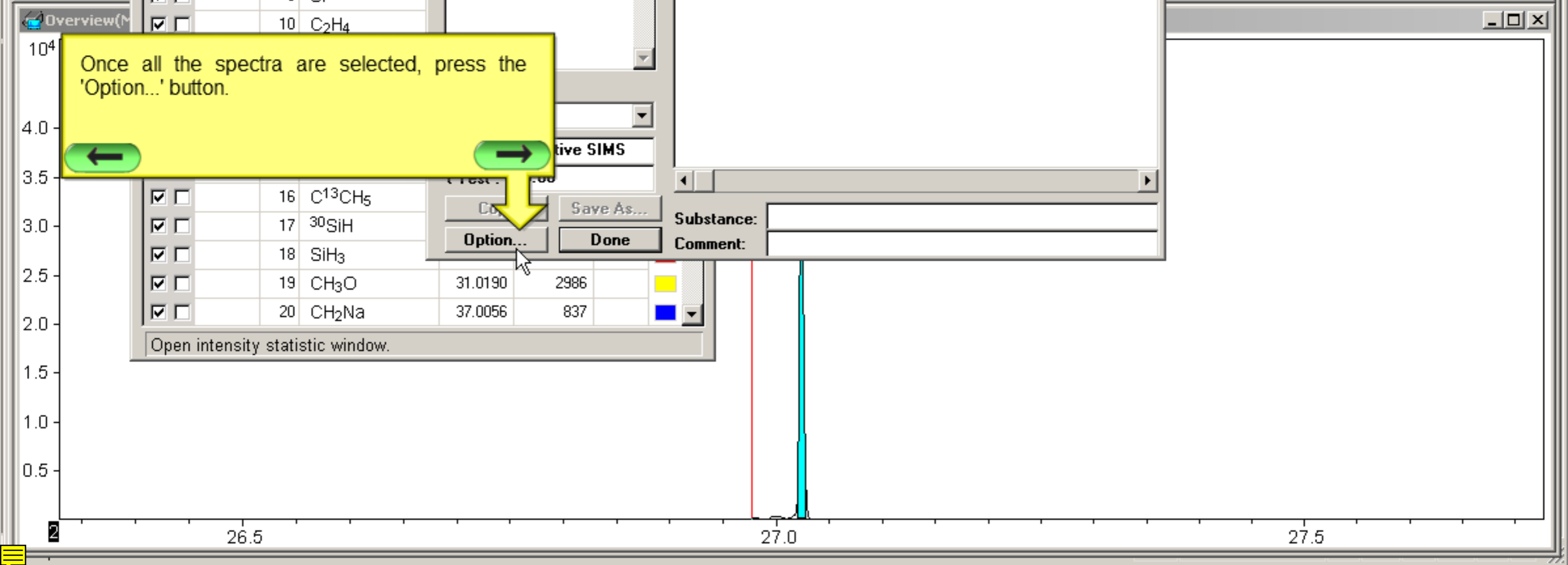
Option... Done

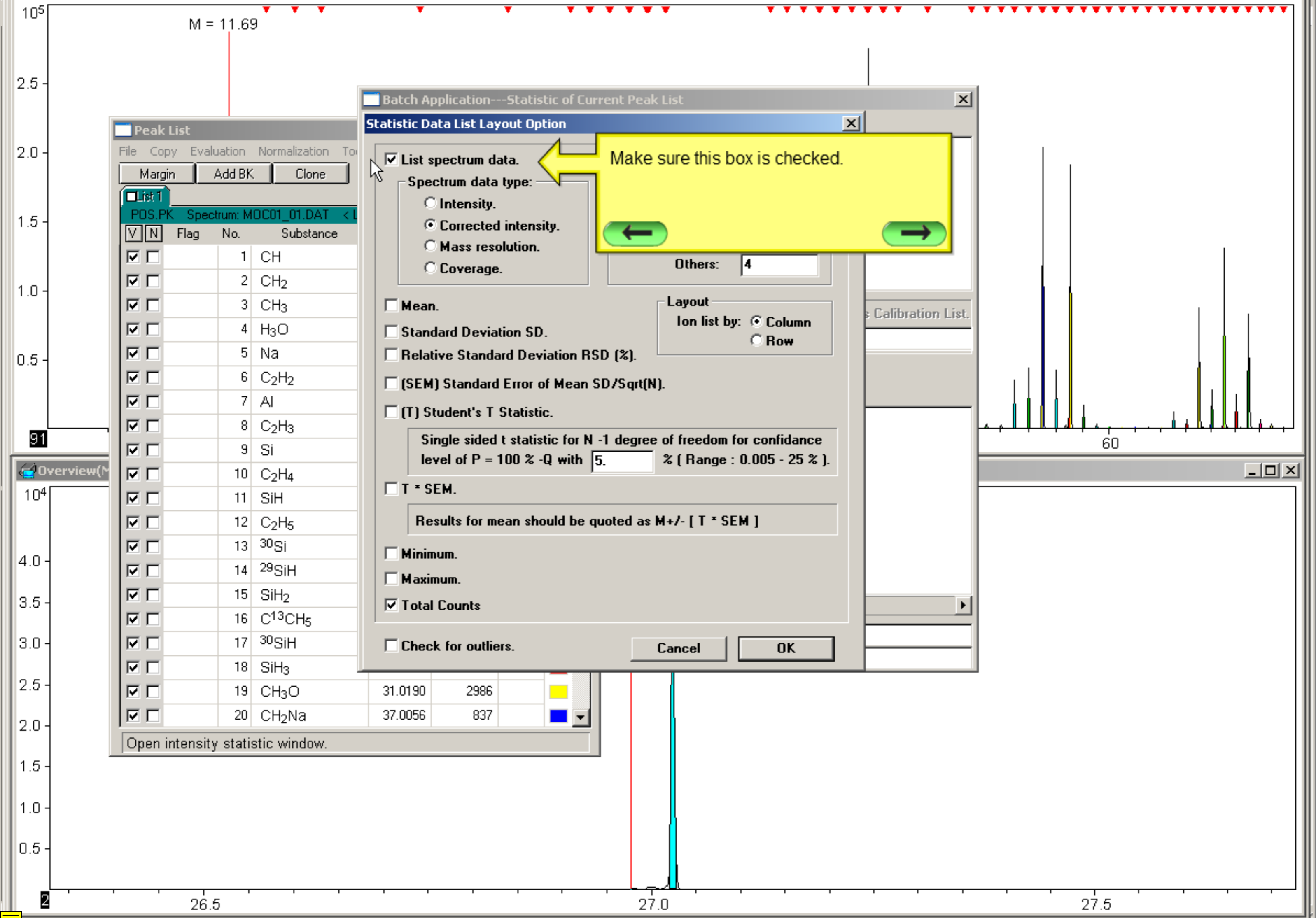


Once all the spectra are selected, press the 'Option...' button.

<input checked="" type="checkbox"/>	<input type="checkbox"/>	16	C <sup>13</sup> CH <sub>5</sub>			
<input checked="" type="checkbox"/>	<input type="checkbox"/>	17	<sup>30</sup> SiH			
<input checked="" type="checkbox"/>	<input type="checkbox"/>	18	SiH <sub>3</sub>			
<input checked="" type="checkbox"/>	<input type="checkbox"/>	19	CH <sub>3</sub> O	31.0190	2986	Yellow
<input checked="" type="checkbox"/>	<input type="checkbox"/>	20	CH <sub>2</sub> Na	37.0056	837	Blue

Open intensity statistic window.





Peak List

File Copy Evaluation Normalization To

Margin Add BK Clone

List 1

POS.PK Spectrum: MOC01\_01.DAT < L

V	N	Flag	No.	Substance				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		1	CH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		2	CH <sub>2</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		3	CH <sub>3</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		4	H <sub>3</sub> O				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		5	Na				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		6	C <sub>2</sub> H <sub>2</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		7	Al				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		8	C <sub>2</sub> H <sub>3</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		9	Si				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		10	C <sub>2</sub> H <sub>4</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		11	SiH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		12	C <sub>2</sub> H <sub>5</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		13	<sup>30</sup> Si				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		14	<sup>29</sup> SiH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		15	SiH <sub>2</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		16	C <sup>13</sup> CH <sub>5</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		17	<sup>30</sup> SiH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		18	SiH <sub>3</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		19	CH <sub>3</sub> O	31.0190	2986		Yellow
<input checked="" type="checkbox"/>	<input type="checkbox"/>		20	CH <sub>2</sub> Na	37.0056	837		Blue

Open intensity statistic window.

Batch Application---Statistic of Current Peak List

Statistic Data List Layout Option

List spectrum data. **Make sure this box is checked.**

Spectrum data type:

- Intensity.
- Corrected intensity.
- Mass resolution.
- Coverage.

Others: 4

Layout

Ion list by:  Column  Row

Mean.

Standard Deviation SD.

Relative Standard Deviation RSD [%].

(SEM) Standard Error of Mean SD/Sqrt(N).

(T) Student's T Statistic.

Single sided t statistic for N -1 degree of freedom for confidence level of P = 100 % - Q with 5. % ( Range : 0.005 - 25 % ).

T \* SEM.

Results for mean should be quoted as M +/- [ T \* SEM ]

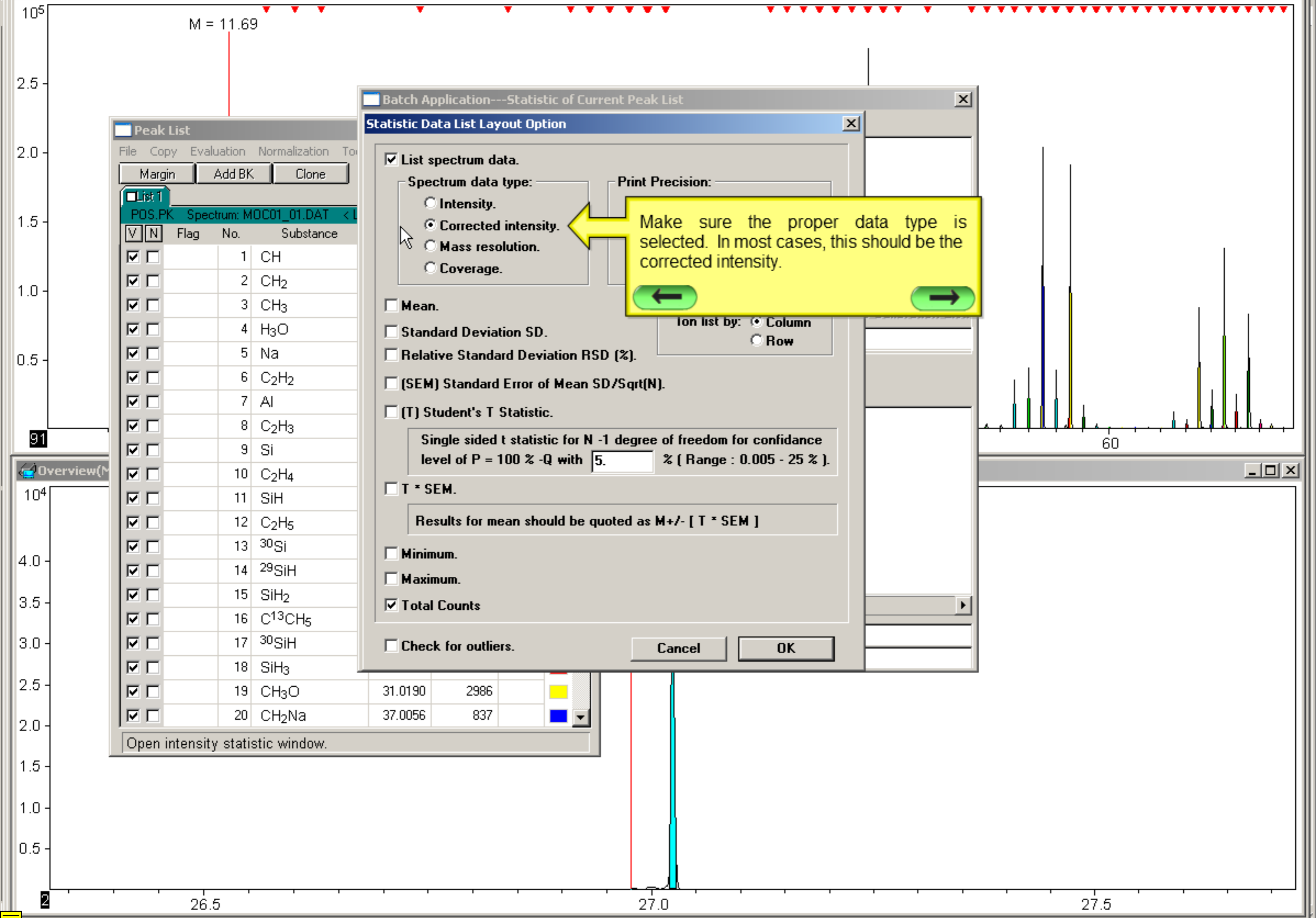
Minimum.

Maximum.

Total Counts

Check for outliers.

Cancel OK



Peak List

File Copy Evaluation Normalization To

Margin Add BK Clone

List 1

POS.PK Spectrum: MOC01\_01.DAT < L

V	N	Flag	No.	Substance				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		1	CH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		2	CH <sub>2</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		3	CH <sub>3</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		4	H <sub>3</sub> O				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		5	Na				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		6	C <sub>2</sub> H <sub>2</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		7	Al				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		8	C <sub>2</sub> H <sub>3</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		9	Si				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		10	C <sub>2</sub> H <sub>4</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		11	SiH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		12	C <sub>2</sub> H <sub>5</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		13	<sup>30</sup> Si				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		14	<sup>29</sup> SiH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		15	SiH <sub>2</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		16	C <sup>13</sup> CH <sub>5</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		17	<sup>30</sup> SiH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		18	SiH <sub>3</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		19	CH <sub>3</sub> O	31.0190	2986		Yellow
<input checked="" type="checkbox"/>	<input type="checkbox"/>		20	CH <sub>2</sub> Na	37.0056	837		Blue

Open intensity statistic window.

Batch Application---Statistic of Current Peak List

Statistic Data List Layout Option

List spectrum data.

Spectrum data type:

- Intensity.
- Corrected intensity.
- Mass resolution.
- Coverage.

Print Precision:

Mean.

Standard Deviation SD.

Relative Standard Deviation RSD [%].

(SEM) Standard Error of Mean SD/Sqrt(N).

(T) Student's T Statistic.

Single sided t statistic for N -1 degree of freedom for confidence level of P = 100 % - Q with 5. % ( Range : 0.005 - 25 % ).

T \* SEM.

Results for mean should be quoted as M+/- [ T \* SEM ]

Minimum.

Maximum.

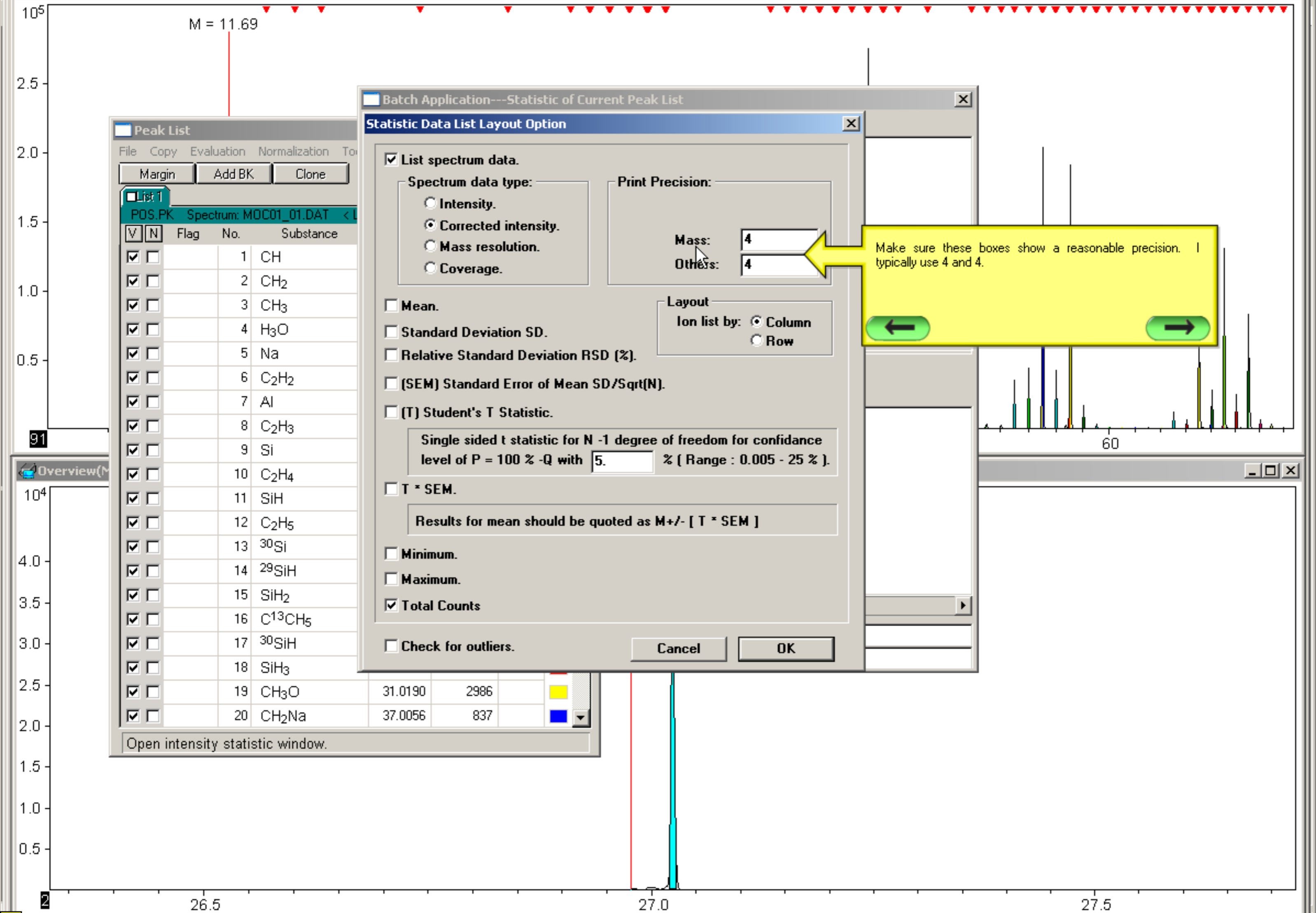
Total Counts

Check for outliers.

Ion list by:  Column  Row

Cancel OK

Make sure the proper data type is selected. In most cases, this should be the corrected intensity.



**Peak List**

File Copy Evaluation Normalization To

Margin Add BK Clone

List 1

POS.PK Spectrum: MOC01\_01.DAT < 1

V	N	Flag	No.	Substance			
<input checked="" type="checkbox"/>	<input type="checkbox"/>		1	CH			
<input checked="" type="checkbox"/>	<input type="checkbox"/>		2	CH <sub>2</sub>			
<input checked="" type="checkbox"/>	<input type="checkbox"/>		3	CH <sub>3</sub>			
<input checked="" type="checkbox"/>	<input type="checkbox"/>		4	H <sub>3</sub> O			
<input checked="" type="checkbox"/>	<input type="checkbox"/>		5	Na			
<input checked="" type="checkbox"/>	<input type="checkbox"/>		6	C <sub>2</sub> H <sub>2</sub>			
<input checked="" type="checkbox"/>	<input type="checkbox"/>		7	Al			
<input checked="" type="checkbox"/>	<input type="checkbox"/>		8	C <sub>2</sub> H <sub>3</sub>			
<input checked="" type="checkbox"/>	<input type="checkbox"/>		9	Si			
<input checked="" type="checkbox"/>	<input type="checkbox"/>		10	C <sub>2</sub> H <sub>4</sub>			
<input checked="" type="checkbox"/>	<input type="checkbox"/>		11	SiH			
<input checked="" type="checkbox"/>	<input type="checkbox"/>		12	C <sub>2</sub> H <sub>5</sub>			
<input checked="" type="checkbox"/>	<input type="checkbox"/>		13	<sup>30</sup> Si			
<input checked="" type="checkbox"/>	<input type="checkbox"/>		14	<sup>29</sup> SiH			
<input checked="" type="checkbox"/>	<input type="checkbox"/>		15	SiH <sub>2</sub>			
<input checked="" type="checkbox"/>	<input type="checkbox"/>		16	C <sup>13</sup> CH <sub>5</sub>			
<input checked="" type="checkbox"/>	<input type="checkbox"/>		17	<sup>30</sup> SiH			
<input checked="" type="checkbox"/>	<input type="checkbox"/>		18	SiH <sub>3</sub>			
<input checked="" type="checkbox"/>	<input type="checkbox"/>		19	CH <sub>3</sub> O	31.0190	2986	Yellow
<input checked="" type="checkbox"/>	<input type="checkbox"/>		20	CH <sub>2</sub> Na	37.0056	837	Blue

Open intensity statistic window.

**Batch Application---Statistic of Current Peak List**

**Statistic Data List Layout Option**

List spectrum data.

Spectrum data type:

- Intensity.
- Corrected intensity.
- Mass resolution.
- Coverage.

Print Precision:

Mass:

Others:

Layout

Ion list by:  Column  Row

Mean.

Standard Deviation SD.

Relative Standard Deviation RSD [%].

(SEM) Standard Error of Mean SD/Sqrt(N).

(T) Student's T Statistic.

Single sided t statistic for N -1 degree of freedom for confidence level of P = 100 % - Q with  % ( Range : 0.005 - 25 % ).

T \* SEM.

Results for mean should be quoted as M+/- [ T \* SEM ]

Minimum.

Maximum.

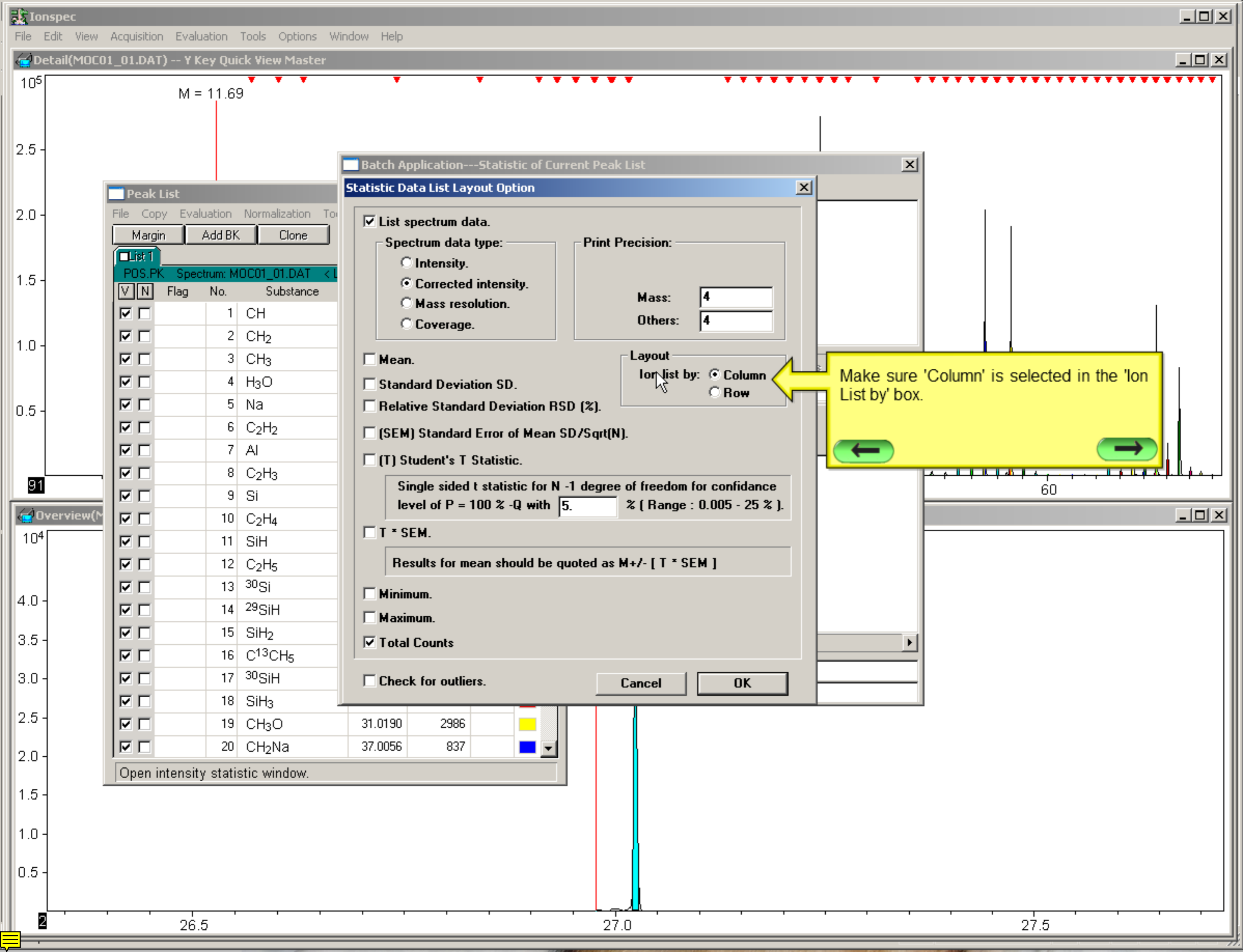
Total Counts

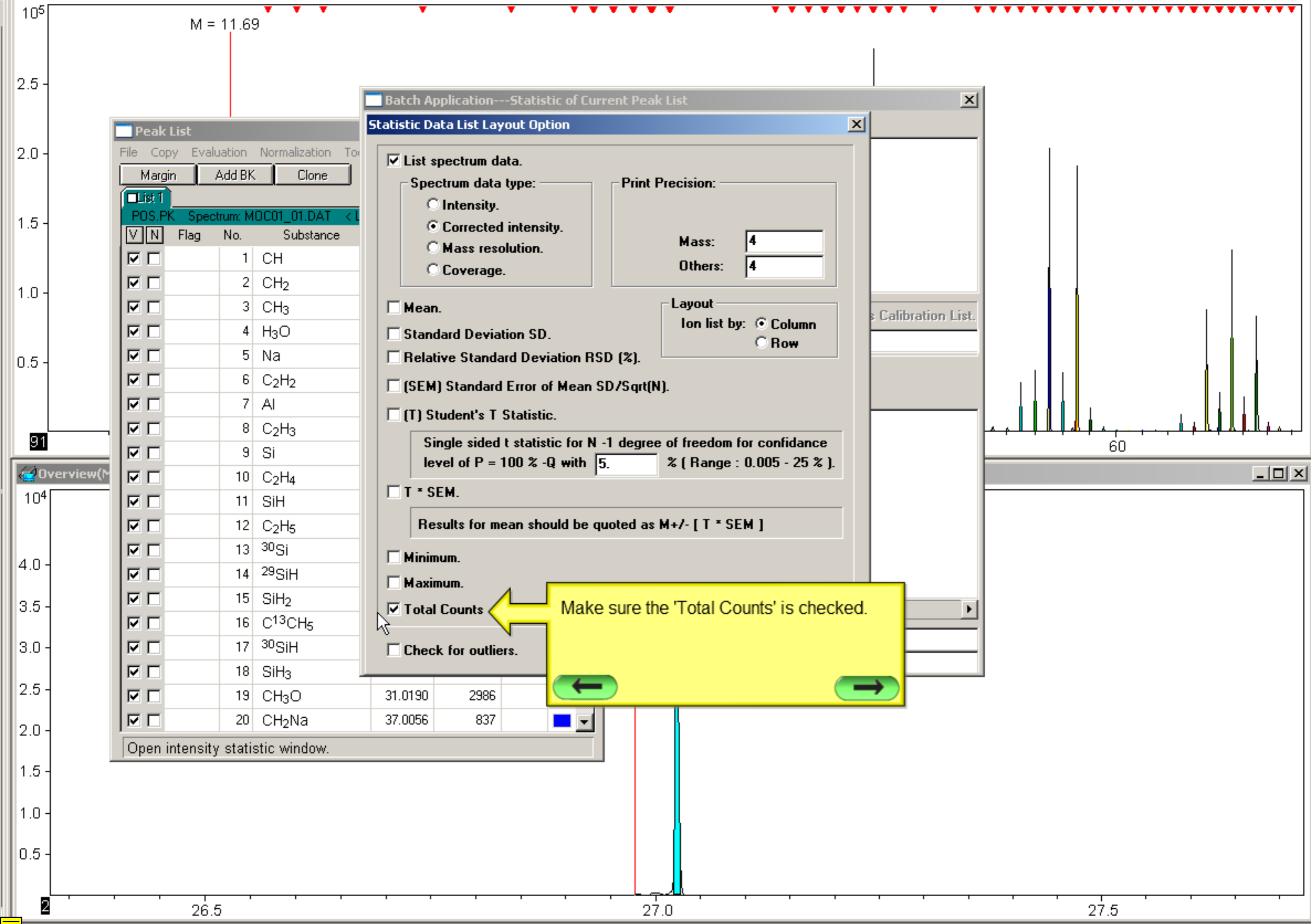
Check for outliers.

Cancel OK

Make sure these boxes show a reasonable precision. I typically use 4 and 4.

← →





Peak List

File Copy Evaluation Normalization To

Margin Add BK Clone

List 1

POS.PK Spectrum: MOC01\_01.DAT < 1

V	N	Flag	No.	Substance		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		1	CH		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		2	CH <sub>2</sub>		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		3	CH <sub>3</sub>		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		4	H <sub>3</sub> O		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		5	Na		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		6	C <sub>2</sub> H <sub>2</sub>		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		7	Al		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		8	C <sub>2</sub> H <sub>3</sub>		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		9	Si		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		10	C <sub>2</sub> H <sub>4</sub>		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		11	SiH		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		12	C <sub>2</sub> H <sub>5</sub>		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		13	<sup>30</sup> Si		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		14	<sup>29</sup> SiH		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		15	SiH <sub>2</sub>		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		16	C <sup>13</sup> CH <sub>5</sub>		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		17	<sup>30</sup> SiH		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		18	SiH <sub>3</sub>		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		19	CH <sub>3</sub> O	31.0190	2986
<input checked="" type="checkbox"/>	<input type="checkbox"/>		20	CH <sub>2</sub> Na	37.0056	837

Open intensity statistic window.

Batch Application--Statistic of Current Peak List

Statistic Data List Layout Option

List spectrum data.

Spectrum data type:

- Intensity.
- Corrected intensity.
- Mass resolution.
- Coverage.

Print Precision:

Mass: 4

Others: 4

Layout

Ion list by:  Column  Row

Mean.

Standard Deviation SD.

Relative Standard Deviation RSD [%].

(SEM) Standard Error of Mean SD/Sqrt(N).

(T) Student's T Statistic.

Single sided t statistic for N -1 degree of freedom for confidence level of P = 100 % - Q with 5. % ( Range : 0.005 - 25 % ).

T \* SEM.

Results for mean should be quoted as M +/- [ T \* SEM ]

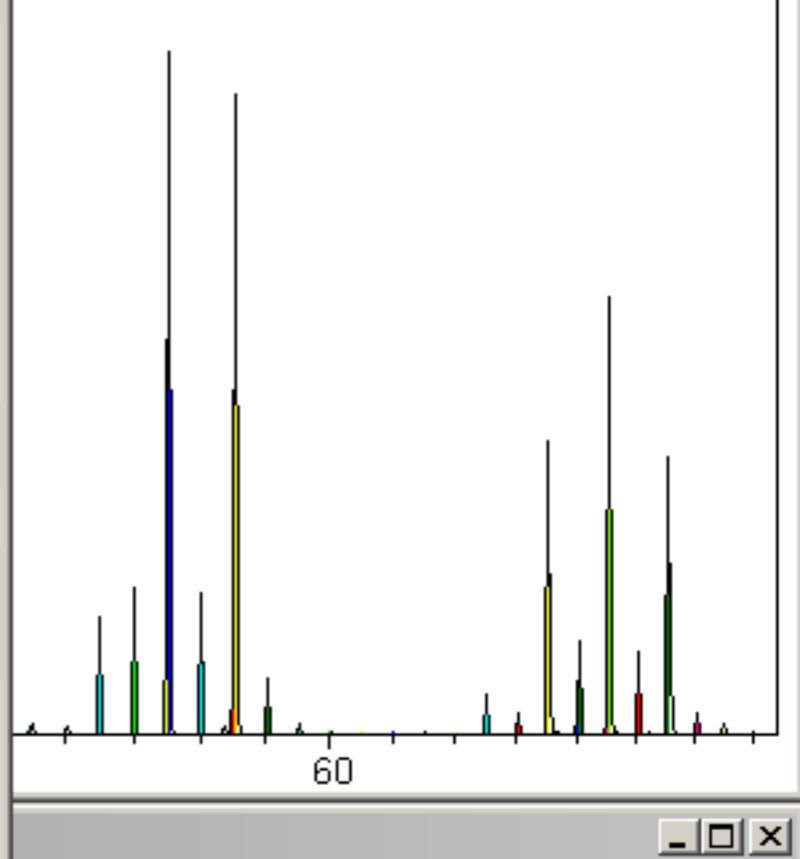
Minimum.

Maximum.

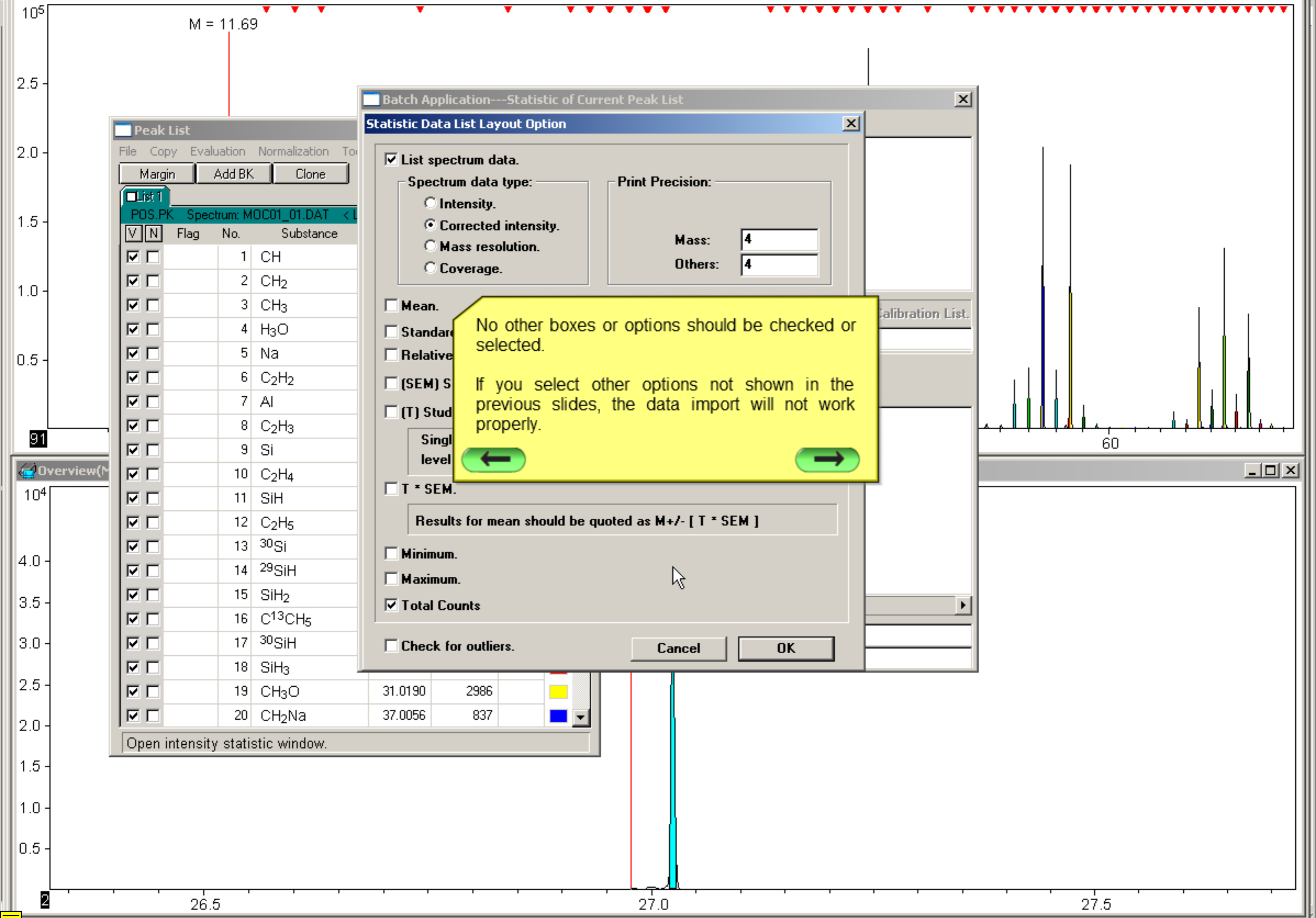
Total Counts

Check for outliers.

Make sure the 'Total Counts' is checked.







Peak List

File Copy Evaluation Normalization To

Margin Add BK Clone

List 1

POS.PK Spectrum: MOC01\_01.DAT <L

V	N	Flag	No.	Substance				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		1	CH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		2	CH <sub>2</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		3	CH <sub>3</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		4	H <sub>3</sub> O				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		5	Na				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		6	C <sub>2</sub> H <sub>2</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		7	Al				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		8	C <sub>2</sub> H <sub>3</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		9	Si				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		10	C <sub>2</sub> H <sub>4</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		11	SiH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		12	C <sub>2</sub> H <sub>5</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		13	<sup>30</sup> Si				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		14	<sup>29</sup> SiH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		15	SiH <sub>2</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		16	C <sup>13</sup> CH <sub>5</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		17	<sup>30</sup> SiH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		18	SiH <sub>3</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		19	CH <sub>3</sub> O	31.0190	2986		Yellow
<input checked="" type="checkbox"/>	<input type="checkbox"/>		20	CH <sub>2</sub> Na	37.0056	837		Blue

Open intensity statistic window.

Batch Application---Statistic of Current Peak List

Statistic Data List Layout Option

List spectrum data.

Spectrum data type:

- Intensity.
- Corrected intensity.
- Mass resolution.
- Coverage.

Print Precision:

Mass:

Others:

Mean.

Standard deviation.

Relative intensity.

(SEM) SEM.

(T) Student's T.

Single level

T \* SEM.

Results for mean should be quoted as M +/- [ T \* SEM ]

Minimum.

Maximum.

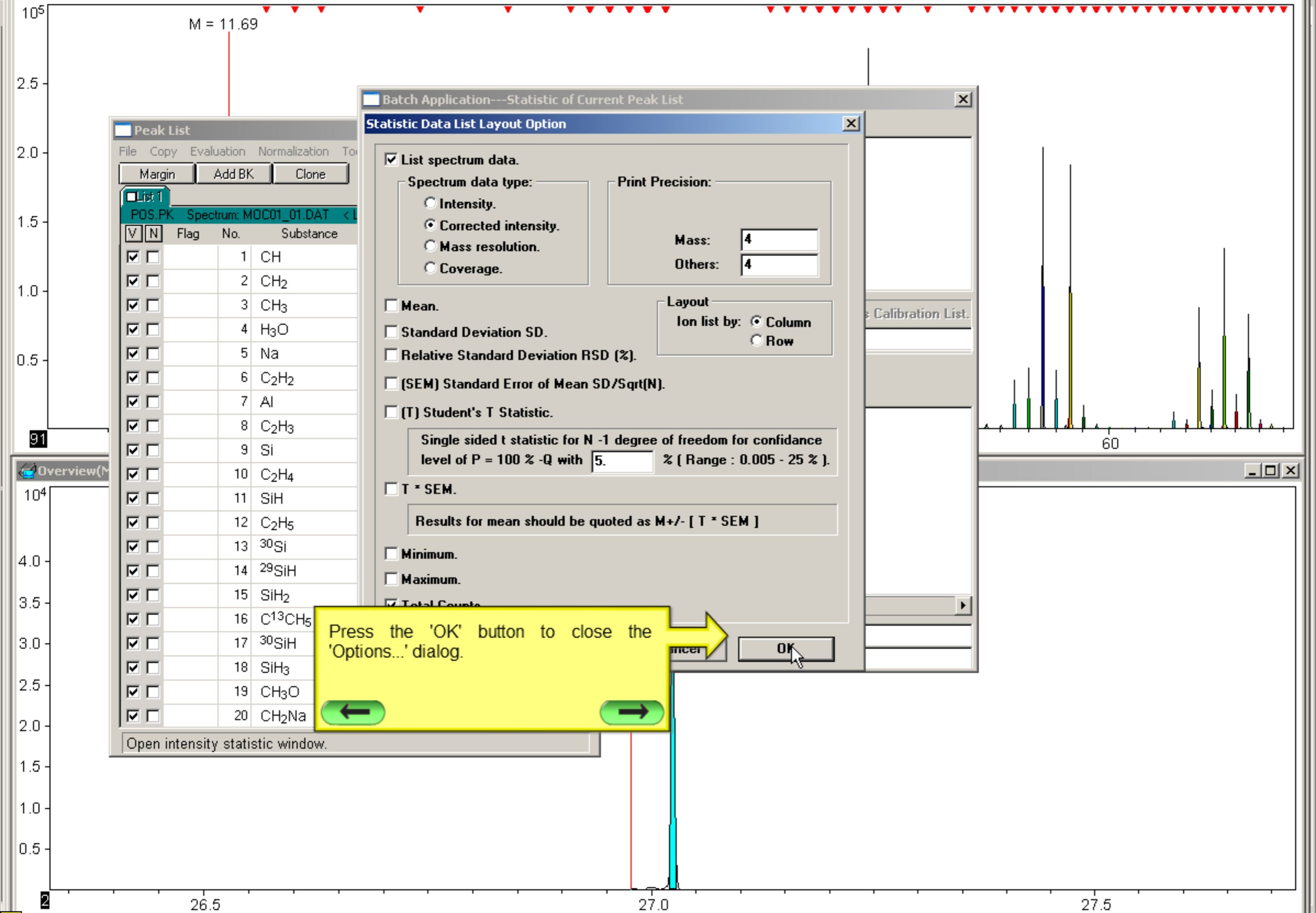
Total Counts

Check for outliers.

Cancel OK

No other boxes or options should be checked or selected.

If you select other options not shown in the previous slides, the data import will not work properly.



Peak List

File Copy Evaluation Normalization To

Margin Add BK Clone

List 1

POS.PK Spectrum: MOC01\_01.DAT < 1

V	N	Flag	No.	Substance
<input checked="" type="checkbox"/>	<input type="checkbox"/>		1	CH
<input checked="" type="checkbox"/>	<input type="checkbox"/>		2	CH <sub>2</sub>
<input checked="" type="checkbox"/>	<input type="checkbox"/>		3	CH <sub>3</sub>
<input checked="" type="checkbox"/>	<input type="checkbox"/>		4	H <sub>3</sub> O
<input checked="" type="checkbox"/>	<input type="checkbox"/>		5	Na
<input checked="" type="checkbox"/>	<input type="checkbox"/>		6	C <sub>2</sub> H <sub>2</sub>
<input checked="" type="checkbox"/>	<input type="checkbox"/>		7	Al
<input checked="" type="checkbox"/>	<input type="checkbox"/>		8	C <sub>2</sub> H <sub>3</sub>
<input checked="" type="checkbox"/>	<input type="checkbox"/>		9	Si
<input checked="" type="checkbox"/>	<input type="checkbox"/>		10	C <sub>2</sub> H <sub>4</sub>
<input checked="" type="checkbox"/>	<input type="checkbox"/>		11	SiH
<input checked="" type="checkbox"/>	<input type="checkbox"/>		12	C <sub>2</sub> H <sub>5</sub>
<input checked="" type="checkbox"/>	<input type="checkbox"/>		13	<sup>30</sup> Si
<input checked="" type="checkbox"/>	<input type="checkbox"/>		14	<sup>29</sup> SiH
<input checked="" type="checkbox"/>	<input type="checkbox"/>		15	SiH <sub>2</sub>
<input checked="" type="checkbox"/>	<input type="checkbox"/>		16	C <sup>13</sup> CH <sub>5</sub>
<input checked="" type="checkbox"/>	<input type="checkbox"/>		17	<sup>30</sup> SiH
<input checked="" type="checkbox"/>	<input type="checkbox"/>		18	SiH <sub>3</sub>
<input checked="" type="checkbox"/>	<input type="checkbox"/>		19	CH <sub>3</sub> O
<input checked="" type="checkbox"/>	<input type="checkbox"/>		20	CH <sub>2</sub> Na

Open intensity statistic window.

Batch Application---Statistic of Current Peak List

Statistic Data List Layout Option

List spectrum data.

Spectrum data type:

- Intensity.
- Corrected intensity.
- Mass resolution.
- Coverage.

Print Precision:

Mass:

Others:

Layout

Ion list by:  Column  Row

Mean.

Standard Deviation SD.

Relative Standard Deviation RSD [%].

(SEM) Standard Error of Mean SD/Sqrt(N).

(T) Student's T Statistic.

Single sided t statistic for N -1 degree of freedom for confidence level of P = 100 % - Q with  % ( Range : 0.005 - 25 % ).

T \* SEM.

Results for mean should be quoted as M +/- [ T \* SEM ]

Minimum.

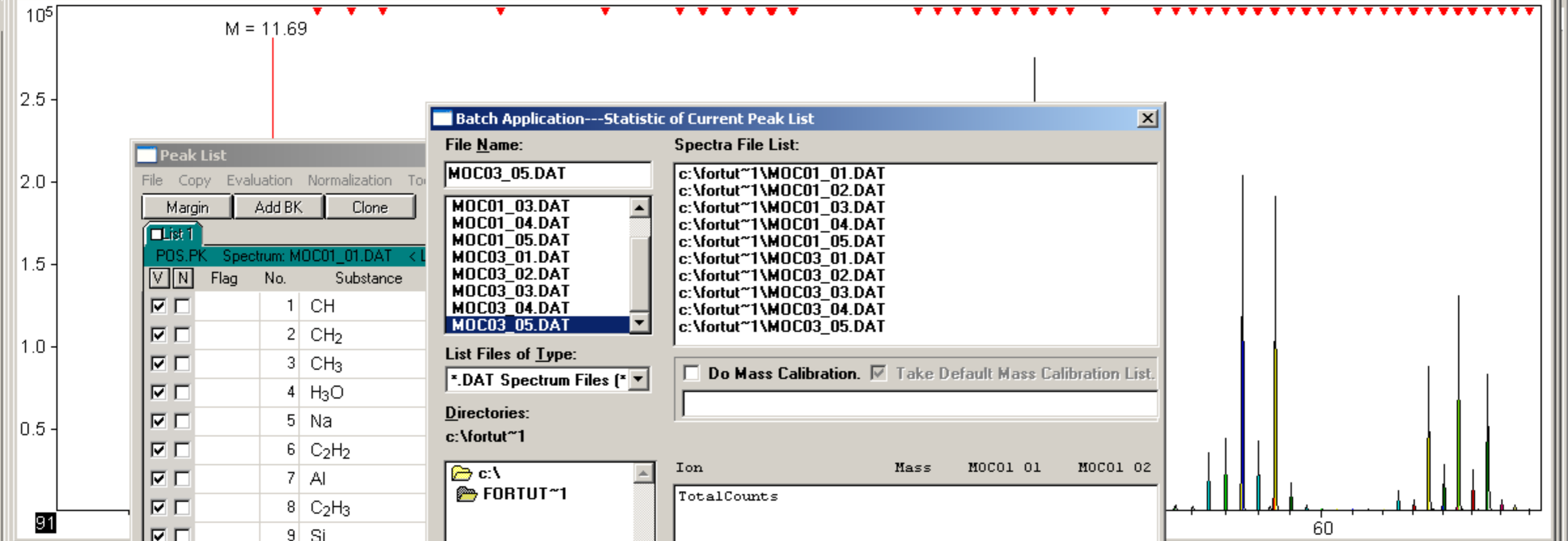
Maximum.

Total Counts

OK

Press the 'OK' button to close the 'Options...' dialog.





Peak List

File Copy Evaluation Normalization To

Margin Add BK Clone

List 1

POS.PK Spectrum: MOC01\_01.DAT

V	N	Flag	No.	Substance		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		1	CH		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		2	CH <sub>2</sub>		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		3	CH <sub>3</sub>		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		4	H <sub>3</sub> O		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		5	Na		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		6	C <sub>2</sub> H <sub>2</sub>		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		7	Al		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		8	C <sub>2</sub> H <sub>3</sub>		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		9	Si		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		10	C <sub>2</sub> H <sub>4</sub>		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		11	SiH		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		12	C <sub>2</sub> H <sub>5</sub>		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		13	<sup>30</sup> Si		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		14	<sup>29</sup> SiH		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		15	SiH <sub>2</sub>		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		16	C <sup>13</sup> CH <sub>5</sub>		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		17	<sup>30</sup> SiH		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		18	SiH <sub>3</sub>		
<input checked="" type="checkbox"/>	<input type="checkbox"/>		19	CH <sub>3</sub> O	31.0190	2986
<input checked="" type="checkbox"/>	<input type="checkbox"/>		20	CH <sub>2</sub> Na	37.0056	837

Open intensity statistic window.

Batch Application---Statistic of Current Peak List

File Name: MOC03\_05.DAT

Spectra File List:

- c:\fortut~1\MOC01\_01.DAT
- c:\fortut~1\MOC01\_02.DAT
- c:\fortut~1\MOC01\_03.DAT
- c:\fortut~1\MOC01\_04.DAT
- c:\fortut~1\MOC01\_05.DAT
- c:\fortut~1\MOC03\_01.DAT
- c:\fortut~1\MOC03\_02.DAT
- c:\fortut~1\MOC03\_03.DAT
- c:\fortut~1\MOC03\_04.DAT
- c:\fortut~1\MOC03\_05.DAT

List Files of Type: \*.DAT Spectrum Files [\*]

Directories: c:\fortut~1

Drives: c:

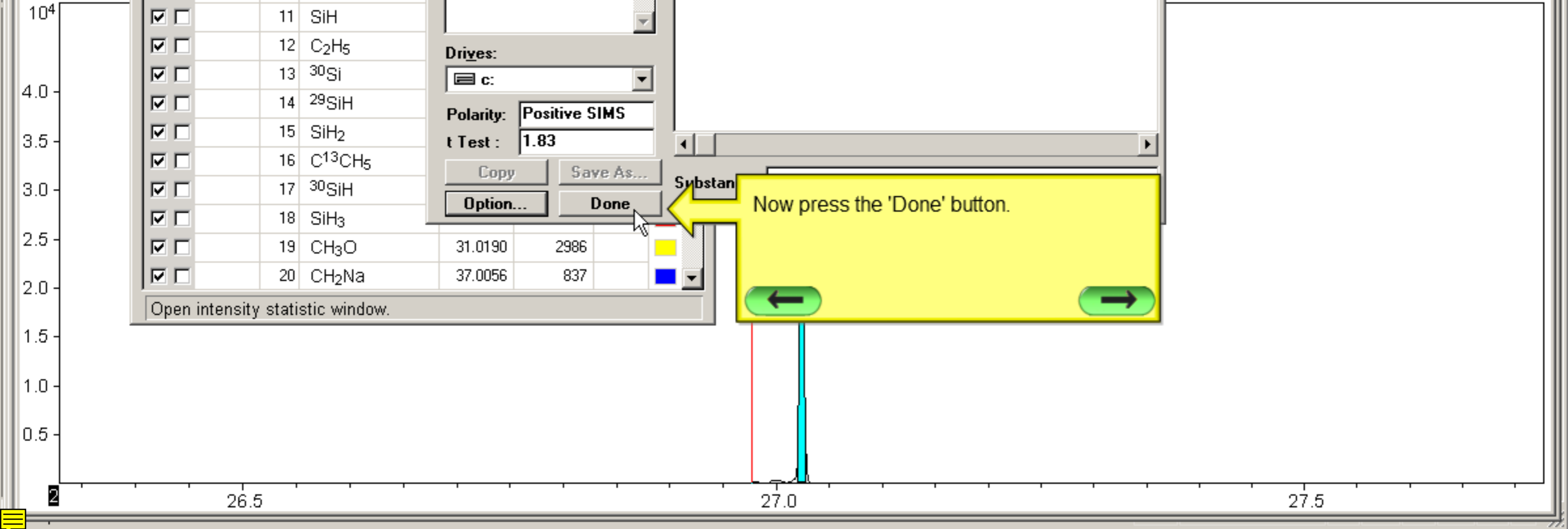
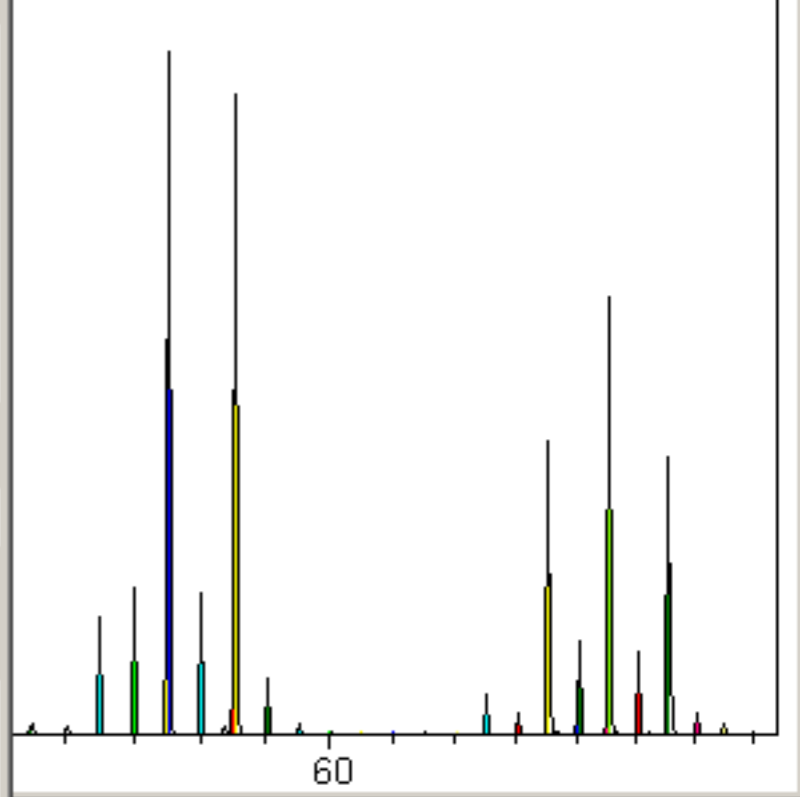
Polarity: Positive SIMS

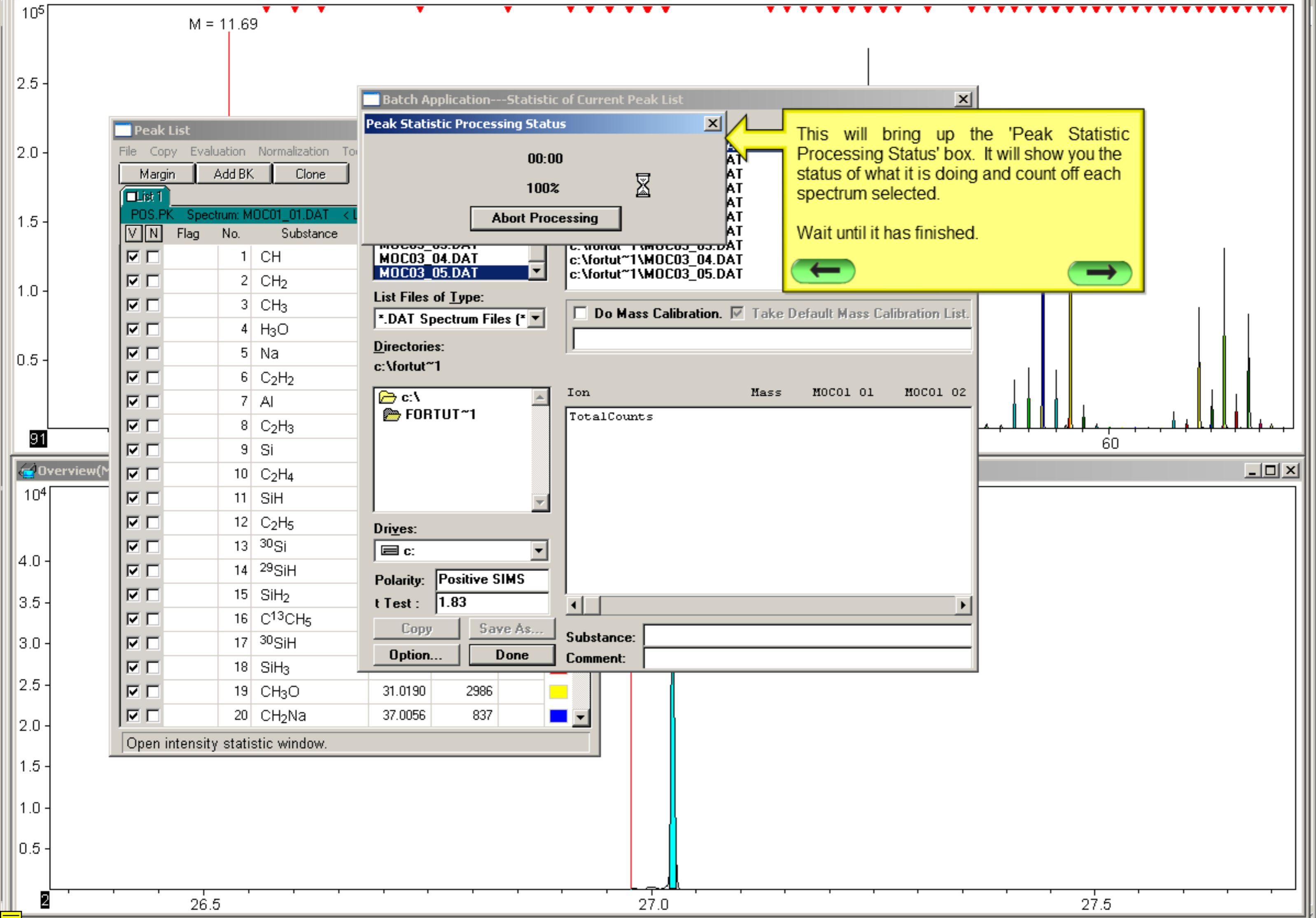
t Test: 1.83

Copy Save As... Option... Done

Ion	Mass	MOC01 01	MOC01 02
TotalCounts			

Now press the 'Done' button.





Peak List

File Copy Evaluation Normalization To

Margin Add BK Clone

List 1

POS.PK Spectrum: MOC01\_01.DAT

V	N	Flag	No.	Substance				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		1	CH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		2	CH <sub>2</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		3	CH <sub>3</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		4	H <sub>3</sub> O				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		5	Na				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		6	C <sub>2</sub> H <sub>2</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		7	Al				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		8	C <sub>2</sub> H <sub>3</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		9	Si				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		10	C <sub>2</sub> H <sub>4</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		11	SiH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		12	C <sub>2</sub> H <sub>5</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		13	<sup>30</sup> Si				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		14	<sup>29</sup> SiH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		15	SiH <sub>2</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		16	C <sup>13</sup> CH <sub>5</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		17	<sup>30</sup> SiH				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		18	SiH <sub>3</sub>				
<input checked="" type="checkbox"/>	<input type="checkbox"/>		19	CH <sub>3</sub> O	31.0190	2986		Yellow
<input checked="" type="checkbox"/>	<input type="checkbox"/>		20	CH <sub>2</sub> Na	37.0056	837		Blue

Open intensity statistic window.

Batch Application---Statistic of Current Peak List

Peak Statistic Processing Status

00:00

100%

Abort Processing

List Files of Type: \*.DAT Spectrum Files (\*)

Directories: c:\fortut~1

Drives: c:

Polarity: Positive SIMS

t Test: 1.83

Substance:

Comment:

Copy Save As... Option... Done

Ion Mass MOC01 01 MOC01 02

TotalCounts

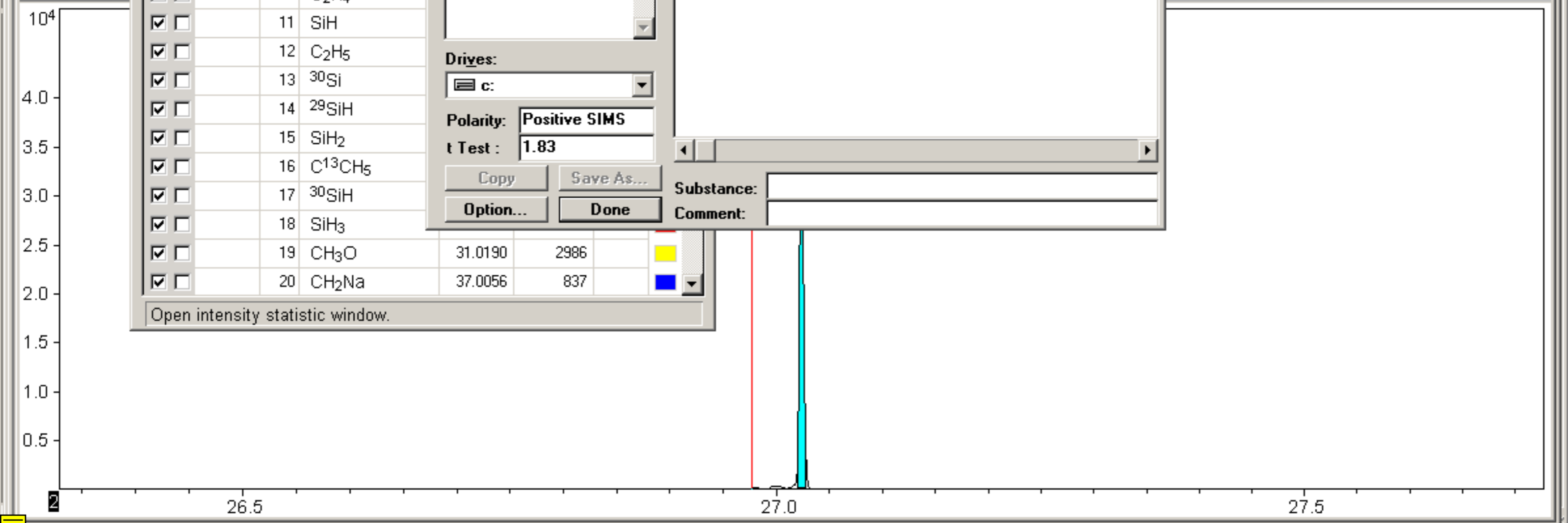
This will bring up the 'Peak Statistic Processing Status' box. It will show you the status of what it is doing and count off each spectrum selected.

Wait until it has finished.

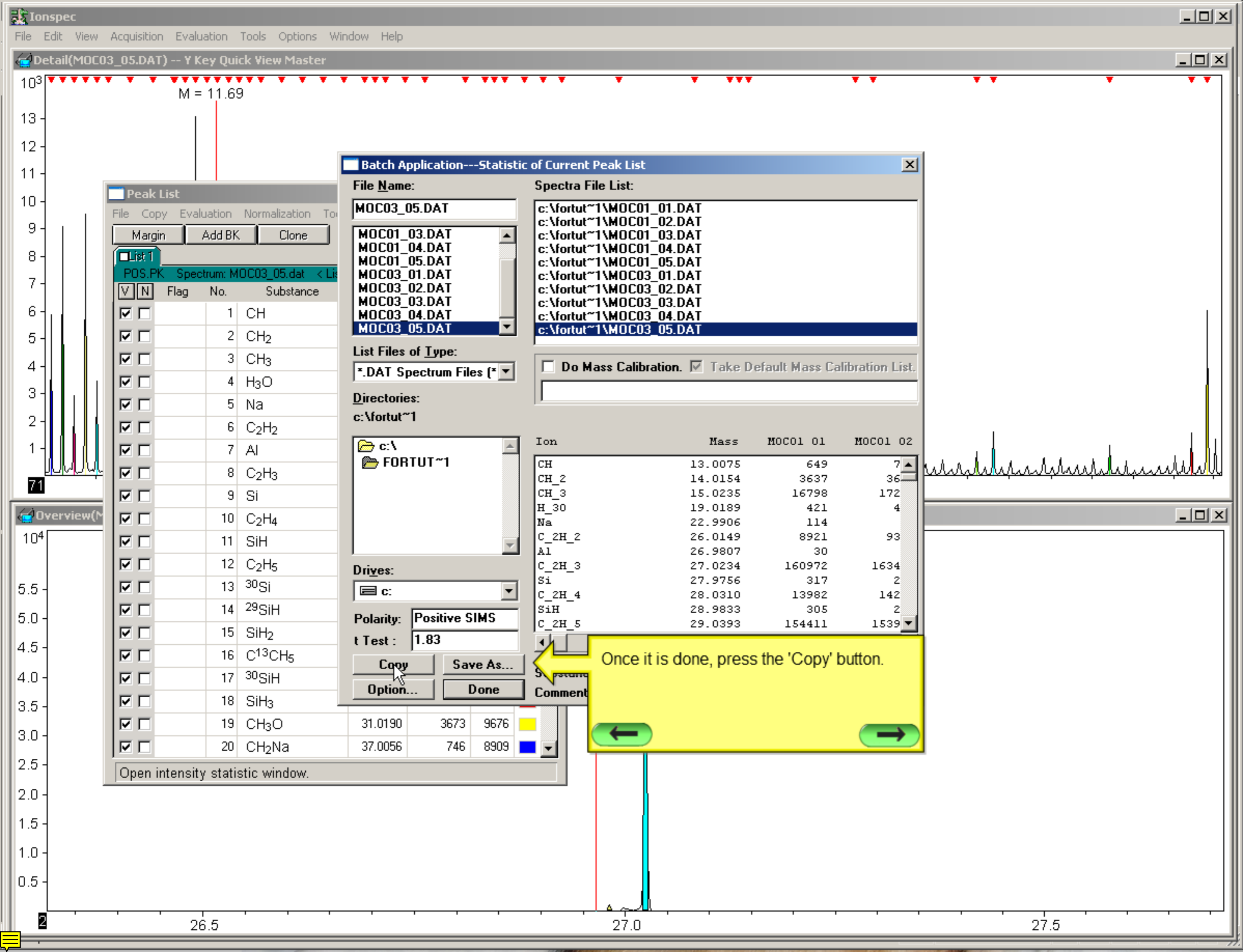


91

Overview(M



2



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1																		
2																		
3																		
4																		
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7																		
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38																		
39																		
40																		
41																		
42																		
43																		
44																		
45																		

Open a spreadsheet and paste the data starting in the first row/column.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	Substance:																	
2	Comment :																	
3	Polarity : Positive SIMS																	
4	Date : 10.11.2010																	
5	Time : 13:09:42																	
6	File(s) : MOC01_01.DAT																	
7	MOC01_02.DAT																	
8	MOC01_03.DAT																	
9	MOC01_04.DAT																	
10	MOC01_05.DAT																	
11	MOC03_01.DAT																	
12	MOC03_02.DAT																	
13	MOC03_03.DAT																	
14	MOC03_04.DAT																	
15	MOC03_05.DAT																	
16	Ion	Mass	MOC01_01	MOC01_02	MOC01_03	MOC01_04	MOC01_05	MOC03_01	MOC03_02	MOC03_03	MOC03_04	MOC03_05	TotalCounts					
17	CH	13.0075	649	727	600	450	429	827	957	973	962	955						
18	CH_2	14.0154	3637	3652	2921	2336	2005	4365	4846	4763	5043	4785						
19	CH_3	15.0235	16798	17225	14481	11674	10776	20996	22684	22824	23978	23233						
20	H_3O	19.0189	421	417	343	331	237	968	1029	1024	1008	1088						
21	Na	22.9906	114	59	49	26	38	1399	1243	1170	1149	1364						
22	C_2H_2	26.0149	8921	9309	8001	6199	5973	11350	12875	12634	12730	13103						
23	Al	26.9807	30	26	19	11	12	2387	2514	2661	2506	3088						
24	C_2H_3	27.0234	160972	163472	143259	114190	110734	199721	214426	215485	217814	227691						
25	Si	27.9756	317	219	157	14	106	56397	61199	57741	63527	70902						
26	C_2H_4	28.031	13982	14213	12345	9510	8912	15944	17155	17316	17141	17879						
27	SiH	28.9833	305	293	167	23	108	57119	63742	60168	65080	72225						
28	C_2H_5	29.0393	154411	153973	136133	110304	104090	157226	166928	170664	163458	168904						
29	<sup>30</sup> Si	29.9722	14	11	5	0	4	1818	2116	1908	2131	2322						
30	<sup>29</sup> SiH	29.9828	14	14	11	2	4	3001	3429	3184	3416	3831						
31	SiH_2	29.9912	14	13	3	0	8	2422	2721	2615	2885	3116						
32	C <sup>13</sup> CH_5	30.0428	3832	3832	3364	2693	2471	4699	5130	4936	5133	5389						
33	<sup>30</sup> SiH	30.9801	8	13	6	1	4	2173	2422	2217	2518	2809						
34	SiH_3	31.0003	21	18	5	3	6	3507	3781	3553	3876	4465						
35	CH_3O	31.019	1333	1354	1226	945	832	3155	3377	3407	3465	3673						
36	CH_2Na	37.0056	430	480	399	300	324	621	739	754	712	746						
37	CH_3Na	38.0139	2984	3010	2527	1970	1925	4109	4382	4349	4737	4682						
38	K	38.9643	8092	8715	10122	8387	6862	53753	60170	70205	71900	74700						
39	C_3H_3	39.0223	65100	66159	56944	45668	43959	71666	76298	72796	73162	77249						
40	Ca	39.9603	97	84	63	37	63	1407	1584	1299	1443	1307						
41	C_3H_4	40.0303	8344	8715	7588	5847	5497	11982	12709	12615	13108	13817						
42	C_2HO	41.002	12230	13196	10909	9437	8351	16219	18235	17269	18981	18934						
43	C_3H_5	41.0386	217861	218907	190576	160395	151292	275246	291714	291195	293492	305962						
44	Unknown	41.99	107	102	81	63	54	4492	5032	4468	5224	5744						
45	C_2H_2O	42.0105	1544	1518	1278	957	821	2295	2370	2473	2402	2631						

Select all the rows containing the header information.

1	Substance:																
2	Comment :																
3	Polarity : Positive SIMS																
4	Date : 10.11.2010																
5	Time : 13:09:42																
6	File(s) : MOC01_01.DAT																
7	MOC01_02.DAT																
8	MOC01_03.DAT																
9	MOC01_04.DAT																
10	MOC01_05.DAT																
11	MOC03_01.DAT																
12	MOC03_02.DAT																
13	MOC03_03.DAT																
14	MOC03_04.DAT																
15	MOC03_05.DAT																

Delete the selected rows.

- Cut
- Copy
- Paste
- Paste Special...
- Insert
- Delete
- Clear Contents
- Format Cells...
- Row Height...
- Hide
- Unhide

	MOC03_01	MOC03_02	MOC03_03	MOC03_04	MOC03_05	TotalCounts											
1	75	64				957	973	962	955								
1	54	363				4846	4763	5043	4785								
1	85	1679				22684	22824	23978	23233								
1	89	42				1029	1024	1008	1088								
2	06	114	59	49	26	38	1399	1243	1170	1149	1364						
2	19	8921	9309	8001	6199	5973	11350	12875	12634	12730	13103						
2	07	30	26	19	11	12	2387	2514	2661	2506	3088						
2	84	160972	163472	143259	114190	110734	199721	214426	215485	217814	227691						
2	56	317	219	157	14	106	56397	61199	57741	63527	70902						
2	81	13982	14213	12345	9510	8912	15944	17155	17316	17141	17879						
2	83	305	293	167	23	108	57119	63742	60168	65080	72225						
2	83	154411	153973	136133	110304	104090	157226	166928	170664	163458	168904						
2	22	14	11	5	0	4	1818	2116	1908	2131	2322						
2	28	14	14	11	2	4	3001	3429	3184	3416	3831						
31	SiH_2	29.9912	14	13	3	0	8	2422	2721	2615	2885	3116					
32	C^13CH_5	30.0428	3832	3832	3364	2693	2471	4699	5130	4936	5133	5389					
33	^30SiH	30.9801	8	13	6	1	4	2173	2422	2217	2518	2809					
34	SiH_3	31.0003	21	18	5	3	6	3507	3781	3553	3876	4465					
35	CH_3O	31.019	1333	1354	1226	945	832	3155	3377	3407	3465	3673					
36	CH_2Na	37.0056	430	480	399	300	324	621	739	754	712	746					
37	CH_3Na	38.0139	2984	3010	2527	1970	1925	4109	4382	4349	4737	4682					
38	K	38.9643	8092	8715	10122	8387	6862	53753	60170	70205	71900	74700					
39	C_3H_3	39.0223	65100	66159	56944	45668	43959	71666	76298	72796	73162	77249					
40	Ca	39.9603	97	84	63	37	63	1407	1584	1299	1443	1307					
41	C_3H_4	40.0303	8344	8715	7588	5847	5497	11982	12709	12615	13108	13817					
42	C_2HO	41.002	12230	13196	10909	9437	8351	16219	18235	17269	18981	18934					
43	C_3H_5	41.0386	217861	218907	190576	160395	151292	275246	291714	291195	293492	305962					
44	Unknown	41.99	107	102	81	63	54	4492	5032	4468	5224	5744					
45	C_2H_2O	42.0105	1544	1518	1278	957	821	2295	2370	2473	2402	2631					



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	lon	Mass	MOC01_0	MOC01_0	MOC01_0	MOC01_0							TotalCounts					
2	CH	13.0075	649	727	600	450							955					
3	CH_2	14.0154	3637	3652	2921	2336							4785					
4	CH_3	15.0235	16798	17225	14481	11674							23233					
5	H_3O	19.0189	421	417	343	331							1088					
6	Na	22.9906	114	59	49	26							1364					
7	C_2H_2	26.0149	8921	9309	8001	6199	5973	11350	12875	12634	12730		13103					
8	Al	26.9807	30	26	19	11	12	2387	2514	2661	2506		3088					
9	C_2H_3	27.0234	160972	163472	143259	114190	110734	199721	214426	215485	217814		227691					
10	Si	27.9756	317	219	157	14	106	56397	61199	57741	63527		70902					
11	C_2H_4	28.031	13982	14213	12345	9510	8912	15944	17155	17316	17141		17879					
12	SiH	28.9833	305	293	167	23	108	57119	63742	60168	65080		72225					
13	C_2H_5	29.0393	154411	153973	136133	110304	104090	157226	166928	170664	163458		168904					
14	<sup>30</sup> Si	29.9722	14	11	5	0	4	1818	2116	1908	2131		2322					
15	<sup>29</sup> SiH	29.9828	14	14	11	2	4	3001	3429	3184	3416		3831					
16	SiH_2	29.9912	14	13	3	0	8	2422	2721	2615	2885		3116					
17	C <sup>13</sup> CH_5	30.0428	3832	3832	3364	2693	2471	4699	5130	4936	5133		5389					
18	<sup>30</sup> SiH	30.9801	8	13	6	1	4	2173	2422	2217	2518		2809					
19	SiH_3	31.0003	21	18	5	3	6	3507	3781	3553	3876		4465					
20	CH_3O	31.019	1333	1354	1226	945	832	3155	3377	3407	3465		3673					
21	CH_2Na	37.0056	430	480	399	300	324	621	739	754	712		746					
22	CH_3Na	38.0139	2984	3010	2527	1970	1925	4109	4382	4349	4737		4682					
23	K	38.9643	8092	8715	10122	8387	6862	53753	60170	70205	71900		74700					
24	C_3H_3	39.0223	65100	66159	56944	45668	43959	71666	76298	72796	73162		77249					
25	Ca	39.9603	97	84	63	37	63	1407	1584	1299	1443		1307					
26	C_3H_4	40.0303	8344	8715	7588	5847	5497	11982	12709	12615	13108		13817					
27	C_2HO	41.002	12230	13196	10909	9437	8351	16219	18235	17269	18981		18934					
28	C_3H_5	41.0386	217861	218907	190576	160395	151292	275246	291714	291195	293492		305962					
29	Unknown	41.99	107	102	81	63	54	4492	5032	4468	5224		5744					
30	C_2H_2O	42.0105	1544	1518	1278	957	821	2295	2370	2473	2402		2631					
31	C_3H_6	42.0457	39557	38921	35316	27436	25695	49622	51063	52611	53047		55709					
32	SiCH3	42.9991	158	137	127	80	93	13253	14304	13448	15217		16708					
33	C_2H_3O	43.0192	4696	4543	4135	3106	2897	8105	8294	8467	8531		9173					
34	C_3H_7	43.055	248655	247109	219552	184767	174484	300864	319759	326088	318696		335491					
35	<sup>29</sup> SiCH_3	43.9983	6	11	11	5	7	624	698	715	788		786					
36	SiCH4	44.0069	10	18	10	12	9	1218	1373	1218	1401		1637					
37	C_2H_4O	44.0254	440	424	384	286	282	846	889	956	932		995					
38	C_2 <sup>13</sup> CH	44.0585	10401	10490	9619	7498	7052	13826	14572	15011	15023		15600					
39	SiHO	44.9792	31	20	9	10	18	2907	3019	2837	3080		3657					
40	CHO_2	44.9965	133	131	106	72	73	836	936	924	955		1020					
41	SiCH_5	45.0157	52	49	36	21	24	4907	5275	5059	5635		6272					
42	C_2H_5O	45.035	1616	1653	1572	1148	1037	3358	3606	3639	3762		3843					
43	SiH_3O	46.9949	13	6	6	4	3	402	390	369	404		461					
44	CH_3O_2	47.0119	95	95	69	75	62	393	480	420	498		539					
45	C_4H_2	50.0137	883	925	720	561	537	1328	1522	1474	1629		1649					

Delete the word 'TotalCounts' from this cell.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	Ion	Mass	MOC01_01	MOC01_02	MOC01_03	MOC01_04	MOC01_05	MOC03_01	MOC03_02	MOC03_03	MOC03_04	MOC03_05						
2	CH	13.0075	649	727	600	450	429	827	957	973	962	955						
3	CH_2	14.0154	3637	3652	2921	2336	2005	4365	4846		5043	4785						
4	CH_3	15.0235	16798	17225	14481	11674	10776	20996	22684	2114	23978	23233						
5	H_3O	19.0189	421	417	343	331	237	968	1029		1008	1088						
6	Na	22.9906	114								1149	1364						
7	C_2H_2	26.0149	8921	93							12730	13103						
8	Al	26.9807	30								2506	3088						
9	C_2H_3	27.0234	160972	1634							217814	227691						
10	Si	27.9756	317	2							63527	70902						
11	C_2H_4	28.031	13982	142							17141	17879						
12	SiH	28.9833	305	293	167	23	108	57119	63742	60168	65080	72225						
13	C_2H_5	29.0393	154411	153973	136133	110304	104090	157226	166928	170664	163458	168904						
14	<sup>30</sup> Si	29.9722	14	11	5	0	4	1818	2116	1908	2131	2322						
15	<sup>29</sup> SiH	29.9828	14	14	11	2	4	3001	3429	3184	3416	3831						
16	SiH_2	29.9912	14	13	3	0	8	2422	2721	2615	2885	3116						
17	C <sup>13</sup> CH_5	30.0428	3832	3832	3364	2693	2471	4699	5130	4936	5133	5389						
18	<sup>30</sup> SiH	30.9801	8	13	6	1	4	2173	2422	2217	2518	2809						
19	SiH_3	31.0003	21	18	5	3	6	3507	3781	3553	3876	4465						
20	CH_3O	31.019	1333	1354	1226	945	832	3155	3377	3407	3465	3673						
21	CH_2Na	37.0056	430	480	399	300	324	621	739	754	712	746						
22	CH_3Na	38.0139	2984	3010	2527	1970	1925	4109	4382	4349	4737	4682						
23	K	38.9643	8092	8715	10122	8387	6862	53753	60170	70205	71900	74700						
24	C_3H_3	39.0223	65100	66159	56944	45668	43959	71666	76298	72796	73162	77249						
25	Ca	39.9603	97	84	63	37	63	1407	1584	1299	1443	1307						
26	C_3H_4	40.0303	8344	8715	7588	5847	5497	11982	12709	12615	13108	13817						
27	C_2HO	41.002	12230	13196	10909	9437	8351	16219	18235	17269	18981	18934						
28	C_3H_5	41.0386	217861	218907	190576	160395	151292	275246	291714	291195	293492	305962						
29	Unknown	41.99	107	102	81	63	54	4492	5032	4468	5224	5744						
30	C_2H_2O	42.0105	1544	1518	1278	957	821	2295	2370	2473	2402	2631						
31	C_3H_6	42.0457	39557	38921	35316	27436	25695	49622	51063	52611	53047	55709						
32	SiCH3	42.9991	158	137	127	80	93	13253	14304	13448	15217	16708						
33	C_2H_3O	43.0192	4696	4543	4135	3106	2897	8105	8294	8467	8531	9173						
34	C_3H_7	43.055	248655	247109	219552	184767	174484	300864	319759	326088	318696	335491						
35	<sup>29</sup> SiCH_3	43.9983	6	11	11	5	7	624	698	715	788	786						
36	SiCH4	44.0069	10	18	10	12	9	1218	1373	1218	1401	1637						
37	C_2H_4O	44.0254	440	424	384	286	282	846	889	956	932	995						
38	C_2 <sup>13</sup> CH	44.0585	10401	10490	9619	7498	7052	13826	14572	15011	15023	15600						
39	SiHO	44.9792	31	20	9	10	18	2907	3019	2837	3080	3657						
40	CHO_2	44.9965	133	131	106	72	73	836	936	924	955	1020						
41	SiCH_5	45.0157	52	49	36	21	24	4907	5275	5059	5635	6272						
42	C_2H_5O	45.035	1616	1653	1572	1148	1037	3358	3606	3639	3762	3843						
43	SiH_3O	46.9949	13	6	6	4	3	402	390	369	404	461						
44	CH_3O_2	47.0119	95	95	69	75	62	393	480	420	498	539						
45	C_4H_2	50.0137	883	925	720	561	537	1328	1522	1474	1629	1649						

Make a note of how many files/spectra are contained in the file. You will need this number when you import the data into the spectragui.



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	Ion	Mass	MOC01_01	MOC01_02	MOC01_03	MOC01_04	MOC01_05	MOC03_01	MOC03_02	MOC03_03	MOC03_04	MOC03_05						
2	CH	13.0075	649	727	600	450	429	827	957	973	962	955						
3	CH_2	14.0154	3637	3652	2921	2336	2005	4365	4846	4763	5043	4785						
4	CH_3	15.0235	16798	17225	14481	11674	10776	20996	22684	22824	23978	23233						
5	H_3O	19.0189	421	417	343	331	237	968	1029	1024	1008	1088						
6	Na	22.9906	114	59	49	26	38	1399	1243	1170	1149	1364						
7	C_2H_2	26.0149	8921	9309	8001	6199	5973	11350	12875	12634	12730	13103						
8	Al	26.9807	30	26	19	11	12	2387	2514	2661	2506	3088						
9	C_2H_3	27.0234	168979	169479	148259	114489	118794	99721	214426	215485	217814	227691						
10	Si	28.0855	56397	61199	57741	63527	70902	15944	17155	17316	17141	17879						
11	C_2H_4	28.0532	57119	63742	60168	65080	72225	57226	166928	170664	163458	168904						
12	SiH	28.9833	1818	2116	1908	2131	2322	3001	3429	3184	3416	3831						
13	C_2H_5	29.0393	2422	2721	2615	2885	3116	4699	5130	4936	5133	5389						
14	^30Si	29.9722	2173	2422	2217	2518	2809	3507	3781	3553	3876	4465						
15	^29SiH	29.9828	3155	3377	3407	3465	3673	4699	5130	4936	5133	5389						
16	SiH_2	29.9912	4699	5130	4936	5133	5389	2173	2422	2217	2518	2809						
17	C^13CH_5	30.0428	21	18	5	3	6	3507	3781	3553	3876	4465						
18	^30SiH	30.9801	1333	1354	1226	945	832	3155	3377	3407	3465	3673						
19	SiH_3	31.0003	430	480	399	300	324	621	739	754	712	746						
20	CH_3O	31.019	2984	3010	2527	1970	1925	4109	4382	4349	4737	4682						
21	CH_2Na	37.0056	8092	8715	10122	8387	6862	53753	60170	70205	71900	74700						
22	CH_3Na	38.0139	65100	66159	56944	45668	43959	71666	76298	72796	73162	77249						
23	K	38.9643	97	84	63	37	63	1407	1584	1299	1443	1307						
24	C_3H_3	39.0223	8344	8715	7588	5847	5497	11982	12709	12615	13108	13817						
25	Ca	39.9603	41.002	12230	13196	10909	9437	8351	16219	18235	17269	18981	18934					
26	C_3H_4	40.0303	41.0386	217861	218907	190576	160395	151292	275246	291714	291195	293492	305962					
27	C_2HO	41.002	41.99	107	102	81	63	54	4492	5032	4468	5224	5744					
28	C_3H_5	41.0386	42.0105	1544	1518	1278	957	821	2295	2370	2473	2402	2631					
29	Unknown	41.99	42.0457	39557	38921	35316	27436	25695	49622	51063	52611	53047	55709					
30	C_2H_2O	42.0105	42.9991	158	137	127	80	93	13253	14304	13448	15217	16708					
31	C_3H_6	42.0457	43.0192	4696	4543	4135	3106	2897	8105	8294	8467	8531	9173					
32	SiCH3	42.9991	43.055	248655	247109	219552	184767	174484	300864	319759	326088	318696	335491					
33	C_2H_3O	43.0192	43.9983	6	11	11	5	7	624	698	715	788	786					
34	C_3H_7	43.055	44.0069	10	18	10	12	9	1218	1373	1218	1401	1637					
35	^29SiCH_3	43.9983	44.0254	440	424	384	286	282	846	889	956	932	995					
36	SiCH4	44.0069	44.0585	10401	10490	9619	7498	7052	13826	14572	15011	15023	15600					
37	C_2H_4O	44.0254	44.9792	31	20	9	10	18	2907	3019	2837	3080	3657					
38	C_2^13CH	44.0585	44.9965	133	131	106	72	73	836	936	924	955	1020					
39	SiHO	44.9792	45.0157	52	49	36	21	24	4907	5275	5059	5635	6272					
40	CHO_2	44.9965	45.035	1616	1653	1572	1148	1037	3358	3606	3639	3762	3843					
41	SiCH_5	45.0157	46.9949	13	6	6	4	3	402	390	369	404	461					
42	C_2H_5O	45.035	47.0119	95	95	69	75	62	393	480	420	498	539					
43	SiH_3O	46.9949	50.0137	883	925	720	561	537	1328	1522	1474	1629	1649					
44	CH_3O_2	47.0119																
45	C_4H_2	50.0137																

Make sure that there are no spaces in the Ion labels.

If you have spaces the file will not import correctly.

← →

	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	MOC01_04	MOC01_05	MOC03_01	MOC03_02	MOC03_03	MOC03_04	MOC03_05						
2			827	957	973	962	955						
3			4365	4846	4763	5043	4785						
4			20996	22684	22824	23978	23233						
5			968	1029	1024	1008	1088						
6			1399	1243	1170	1149	1364						
7			11350	12875	12634	12730	13103						
8			2387	2514	2661	2506	3088						
9			114190	110734	199721	214426	215485	217814	227691				
10			14	106	56397	61199	57741	63527	70902				
11			9510	8912	15944	17155	17316	17141	17879				
12			23	108	57119	63742	60168	65080	72225				
13			110304	104090	157226	166928	170664	163458	168904				
14			0	4	1818	2116	1908	2131	2322				
15			2	4	3001	3429	3184	3416	3831				
16			0	8	2422	2721	2615	2885	3116				
17			2693	2471	4699	5130	4936	5133	5389				
18			1	4	2173	2422	2217	2518	2809				
19			3	6	3507	3781	3553	3876	4465				
20			945	832	3155	3377	3407	3465	3673				
21			300	324	621	739	754	712	746				
22			1970	1925	4109	4382	4349	4737	4682				
23	K	38.9643	8092	8715	10122	8387	6862	53753	60170	70205	71900	74700	
24	C_3H_3	39.0223	65100	66159	56944	45668	43959	71666	76298	72796	73162	77249	
25	Ca	39.9603	97	84	63	37	63	1407	1584	1299	1443	1307	
26	C_3H_4	40.0303	8344	8715	7588	5847	5497	11982	12709	12615	13108	13817	
27	C_2HO	41.002	12230	13196	10909	9437	8351	16219	18235	17269	18981	18934	
28	C_3H_5	41.0386	217861	218907	190576	160395	151292	275246	291714	291195	293492	305962	
29	Unknown	41.99	107	102	81	63	54	4492	5032	4468	5224	5744	
30	C_2H_2O	42.0105	1544	1518	1278	957	821	2295	2370	2473	2402	2631	
31	C_3H_6	42.0457	39557	38921	35316	27436	25695	49622	51063	52611	53047	55709	
32	SiCH3	42.9991	158	137	127	80	93	13253	14304	13448	15217	16708	
33	C_2H_3O	43.0192	4696	4543	4135	3106	2897	8105	8294	8467	8531	9173	
34	C_3H_7	43.055	248655	247109	219552	184767	174484	300864	319759	326088	318696	335491	
35	*29SiCH_3	43.9983	6	11	11	5	7	624	698	715	788	786	
36	SiCH4	44.0069	10	18	10	12	9	1218	1373	1218	1401	1637	
37	C_2H_4O	44.0254	440	424	384	286	282	846	889	956	932	995	
38	C_2*13CH	44.0585	10401	10490	9619	7498	7052	13826	14572	15011	15023	15600	
39	SiHO	44.9792	31	20	9	10	18	2907	3019	2837	3080	3657	
40	CHO_2	44.9965	133	131	106	72	73	836	936	924	955	1020	
41	SiCH_5	45.0157	52	49	36	21	24	4907	5275	5059	5635	6272	
42	C_2H_5O	45.035	1616	1653	1572	1148	1037	3358	3606	3639	3762	3843	
43	SiH_3O	46.9949	13	6	6	4	3	402	390	369	404	461	
44	CH_3O_2	47.0119	95	95	69	75	62	393	480	420	498	539	
45	C_4H_2	50.0137	883	925	720	561	537	1328	1522	1474	1629	1649	

Now go to the 'File' menu and choose 'Save As...'



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	Ion	Mass	MOC01_0	MOC01_02	MOC01_03	MOC01_04	MOC01_05	MOC03_0	MOC03_02	MOC03_03	MOC03_04	MOC03_05						
2	CH	13.0075	649	727	600	450	429	827	957	973	962	955						
3	CH_2	14.0154	3637	3652	2921	2336	2005	4365	4846	4763	5043	4785						
4	CH_3	15.0235	16798	17225	14481	11674	10776	20996	22684	22824	23978	23233						
5	H_3O	19.0189	421	417	343	331	237	968	1029	1024	1008	1088						
6	Na	22.9906	114	59	49	26	38	1399	1243	1170	1149	1364						
7	C_2H_2	26.0149	8921	9309	8001	6199	5973	11350	12875	12634	12730	13103						
8	Al	26.9807	30	26	19	11	12	2387	2514	2661	2506	3088						
9	C_2H_3	27.0234	160972	163472	143259	114190	110734	199721	214426	215485	217814	227691						
10	Si	27.9756	317	219	157	14	106	56397	61199	57741	63527	70902						
11	C_2H_4	28.031	13982	14213	12345	9510	8912	15944	17155	17316	17141	17879						
12	SiH	28.9833	305	293	167	23	108	57119	63742	60168	65080	72225						
13	C_2H_5	29.0393	154411	153973	136133	110304	104090	157226	166928	170664	163458	168904						
14	<sup>30</sup> Si	29.9722	14	11	5	0	4	1818	2116	1908	2131	2322						
15	<sup>29</sup> SiH	29.9828	14	14	11	2	4	3001	3429	3184	3416	3831						
16	SiH_2	29.9912	14	13	3	0												
17	C <sup>13</sup> CH_5	30.0428	3832	3832	3364	2693												
18	<sup>30</sup> SiH	30.9801	8	13	6	1												
19	SiH_3	31.0003	21	18	5	3												
20	CH_3O	31.019	1333	1354	1226	945												
21	CH_2Na	37.0056	430	480	399	300												
22	CH_3Na	38.0139	2984	3010	2527	1970												
23	K	38.9643	8092	8715	10122	8387												
24	C_3H_3	39.0223	65100	66159	56944	45668	4											
25	Ca	39.9603	97	84	63	37												
26	C_3H_4	40.0303	8344	8715	7588	5847												
27	C_2HO	41.002	12230	13196	10909	9437												
28	C_3H_5	41.0386	217861	218907	190576	160395	15											
29	Unknown	41.99	107	102	81	63												
30	C_2H_2O	42.0105	1544	1518	1278	957												
31	C_3H_6	42.0457	39557	38921	35316	27436	2											
32	SiCH3	42.9991	158	137	127	80												
33	C_2H_3O	43.0192	4696	4543	4135	3106												
34	C_3H_7	43.055	248655	247109	219552	184767	17											
35	<sup>29</sup> SiCH_3	43.9983	6	11	11	5												
36	SiCH4	44.0069	10	18	10	12												
37	C_2H_4O	44.0254	440	424	384	286												
38	C_2 <sup>13</sup> CH	44.0585	10401	10490	9619	7498												
39	SiHO	44.9792	31	20	9	10	18	2907	3019	2837	3080	3657						
40	CHO_2	44.9965	133	131	106	72	73	836	936	924	955	1020						
41	SiCH_5	45.0157	52	49	36	21	24	4907	5275	5059	5635	6272						
42	C_2H_5O	45.035	1616	1653	1572	1148	1037	3358	3606	3639	3762	3843						
43	SiH_3O	46.9949	13	6	6	4	3	402	390	369	404	461						
44	CH_3O_2	47.0119	95	95	69	75	62	393	480	420	498	539						
45	C_4H_2	50.0137	883	925	720	561	537	1328	1522	1474	1629	1649						

**Save As**

Save in: My Documents

- Downloads
- gegl-0.0
- My Music
- My Pictures
- My Tofdata

History

My Documents

File name: Book1.xls

Save as type: Microsoft Excel Workbook (\*.xls)

Save Cancel

Change the file type to 'Text Tab Delimited (\*.TXT)'

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	Ion	Mass	MOC01_0	MOC01_0	MOC01_0	MOC01_0	MOC01_0	MOC03_0	MOC03_0	MOC03_0	MOC03_0	MOC03_0						
2	CH	13.0075	649	727	600	450	429	827	957	973	962	955						
3	CH_2	14.0154	3637	3652	2921	2336	2005	4365	4846	4763	5043	4785						
4	CH_3	15.0235	16798	17225	14481	11674	10776	20996	22684	22824	23978	23233						
5	H_3O	19.0189	421	417	343	331	237	968	1029	1024	1008	1088						
6	Na	22.9906	114	59	49	26	38	1399	1243	1170	1149	1364						
7	C_2H_2	26.0149	8921	9309	8001	6199	5973	11350	12875	12634	12730	13103						
8	Al	26.9807	30	26	19	11	12	2387	2514	2661	2506	3088						
9	C_2H_3	27.0234	160972	163472	143259	114190	110734	199721	214426	215485	217814	227691						
10	Si	27.9756	317	219	157							70902						
11	C_2H_4	28.031	13982	14213	12345							17879						
12	SiH	28.9833	305	293	167							72225						
13	C_2H_5	29.0393	154411	153973	136133							168904						
14	<sup>30</sup> Si	29.9722	14	11	5							2322						
15	<sup>29</sup> SiH	29.9828	14	14	11							3831						
16	SiH_2	29.9912	14	13	3													
17	C <sup>13</sup> CH_5	30.0428	3832	3832	3364	2693												
18	<sup>30</sup> SiH	30.9801	8	13	6	1												
19	SiH_3	31.0003	21	18	5	3												
20	CH_3O	31.019	1333	1354	1226	945												
21	CH_2Na	37.0056	430	480	399	300												
22	CH_3Na	38.0139	2984	3010	2527	1970												
23	K	38.9643	8092	8715	10122	8387												
24	C_3H_3	39.0223	65100	66159	56944	45668	4											
25	Ca	39.9603	97	84	63	37												
26	C_3H_4	40.0303	8344	8715	7588	5847												
27	C_2HO	41.002	12230	13196	10909	9437												
28	C_3H_5	41.0386	217861	218907	190576	160395	15											
29	Unknown	41.99	107	102	81	63												
30	C_2H_2O	42.0105	1544	1518	1278	957												
31	C_3H_6	42.0457	39557	38921	35316	27436	2											
32	SiCH3	42.9991	158	137	127	80												
33	C_2H_3O	43.0192	4696	4543	4135	3106												
34	C_3H_7	43.055	248655	247109	219552	184767	17											
35	<sup>29</sup> SiCH_3	43.9983	6	11	11	5												
36	SiCH4	44.0069	10	18	10	12												
37	C_2H_4O	44.0254	440	424	384	286												
38	C_2 <sup>13</sup> CH	44.0585	10401	10490	9619	7498												
39	SiHO	44.9792	31	20	9	10	18	2907	3019	2837	3080	3657						
40	CHO_2	44.9965	133	131	106	72	73	836	936	924	955	1020						
41	SiCH_5	45.0157	52	49	36	21	24	4907	5275	5059	5635	6272						
42	C_2H_5O	45.035	1616	1653	1572	1148	1037	3358	3606	3639	3762	3843						
43	SiH_3O	46.9949	13	6	6	4	3	402	390	369	404	461						
44	CH_3O_2	47.0119	95	95	69	75	62	393	480	420	498	539						
45	C_4H_2	50.0137	883	925	720	561	537	1328	1522	1474	1629	1649						

Choose where you want to save the file.

**Save As**

Save in: graham's Documents

- Desktop
- My Computer
- graham's Documents
- Shared Documents
- Local Disk (C:)
- DVD-RAM Drive (D:)
- home on 'NB File Server (fs.n...)
- My Network Places
- My Documents
- FTP Locations
- Add/Modify FTP Locations

File name: Book1.txt

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

Save Cancel

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	Ion	Mass	MOC01_0	MOC01_02	MOC01_03	MOC01_04	MOC01_05	MOC03_0	MOC03_02	MOC03_03	MOC03_04	MOC03_05						
2	CH	13.0075	649	727	600	450	429	827	957	973	962	955						
3	CH_2	14.0154	3637	3652	2921	2336	2005	4365	4846	4763	5043	4785						
4	CH_3	15.0235	16798	17225	14481	11674	10776	20996	22684	22824	23978	23233						
5	H_3O	19.0189	421	417	343	331	237	968	1029	1024	1008	1088						
6	Na	22.9906	114	59	49	26	38	1399	1243	1170	1149	1364						
7	C_2H_2	26.0149	8921	9309	8001	6199	5973	11350	12875	12634	12730	13103						
8	Al	26.9807	30	26	19	11	12	2387	2514	2661	2506	3088						
9	C_2H_3	27.0234	160972	163472	143259	114190	110734	199721	214426	215485	217814	227691						
10	Si	27.9756	317	219	157	14	106	56397	61199	57741	63527	70902						
11	C_2H_4	28.031	13982	14213	12345	9510	8912	15944	17155	17316	17141	17879						
12	SiH	28.9833	305	293	167	23	108	57119	63742	60168	65080	72225						
13	C_2H_5	29.0393	154411	153973	136133	110304	104090	157226	166928	170664	163458	168904						
14	<sup>30</sup> Si	29.9722	14	11	5	0	4	1818	2116	1908	2131	2322						
15	<sup>29</sup> SiH	29.9828	14	14	11	2	4	3001	3429	3184	3416	3831						
16	SiH_2	29.9912	14	13	3	0												
17	C <sup>13</sup> CH_5	30.0428	3832	3832	3364	2693												
18	<sup>30</sup> SiH	30.9801	8	13	6	1												
19	SiH_3	31.0003	21	18	5	3												
20	CH_3O	31.019	1333	1354	1226	945												
21	CH_2Na	37.0056	430	480	399	300												
22	CH_3Na	38.0139	2984	3010	2527	1970												
23	K	38.9643	8092	8715	10122	8387												
24	C_3H_3	39.0223	65100	66159	56944	45668	4											
25	Ca	39.9603	97	84	63	37												
26	C_3H_4	40.0303	8344	8715	7588	5847												
27	C_2HO	41.002	12230	13196	10													
28	C_3H_5	41.0386	217861	218907	190													
29	Unknown	41.99	107	102														
30	C_2H_2O	42.0105	1544	1518	1													
31	C_3H_6	42.0457	39557	38921	35													
32	SiCH3	42.9991	158	137														
33	C_2H_3O	43.0192	4696	4543	4135	3106												
34	C_3H_7	43.055	248655	247109	219552	184767	17											
35	<sup>29</sup> SiCH_3	43.9983	6	11	11	5												
36	SiCH4	44.0069	10	18	10	12												
37	C_2H_4O	44.0254	440	424	384	286												
38	C_2 <sup>13</sup> CH	44.0585	10401	10490	9619	7498												
39	SiHO	44.9792	31	20	9	10	18	2907	3019	2837	3080	3657						
40	CHO_2	44.9965	133	131	106	72	73	836	936	924	955	1020						
41	SiCH_5	45.0157	52	49	36	21	24	4907	5275	5059	5635	6272						
42	C_2H_5O	45.035	1616	1653	1572	1148	1037	3358	3606	3639	3762	3843						
43	SiH_3O	46.9949	13	6	6	4	3	402	390	369	404	461						
44	CH_3O_2	47.0119	95	95	69	75	62	393	480	420	498	539						
45	C_4H_2	50.0137	883	925	720	561	537	1328	1522	1474	1629	1649						

**Save As**

Save in: fortutorial

History

My Documents

Favorites

My Network Places

File name: Book1.txt

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

Save

Cancel

Give the file a name.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	Ion	Mass	MOC01_0	MOC01_0	MOC01_0	MOC01_0	MOC01_0	MOC03_0	MOC03_0	MOC03_0	MOC03_0	MOC03_0						
2	CH	13.0075	649	727	600	450	429	827	957	973	962	955						
3	CH_2	14.0154	3637	3652	2921	2336	2005	4365	4846	4763	5043	4785						
4	CH_3	15.0235	16798	17225	14481	11674	10776	20996	22684	22824	23978	23233						
5	H_3O	19.0189	421	417	343	331	237	968	1029	1024	1008	1088						
6	Na	22.9906	114	59	49	26	38	1399	1243	1170	1149	1364						
7	C_2H_2	26.0149	8921	9309	8001	6199	5973	11350	12875	12634	12730	13103						
8	Al	26.9807	30	26	19	11	12	2387	2514	2661	2506	3088						
9	C_2H_3	27.0234	160972	163472	143259	114190	110734	199721	214426	215485	217814	227691						
10	Si	27.9756	317	219	157	14	106	56397	61199	57741	63527	70902						
11	C_2H_4	28.031	13982	14213	12345	9510	8912	15944	17155	17316	17141	17879						
12	SiH	28.9833	305	293	167	23	108	57119	63742	60168	65080	72225						
13	C_2H_5	29.0393	154411	153973	136133	110304	104090	157226	166928	170664	163458	168904						
14	<sup>30</sup> Si	29.9722	14	11	5	0	4	1818	2116	1908	2131	2322						
15	<sup>29</sup> SiH	29.9828	14	14	11	2	4	3001	3429	3184	3416	3831						
16	SiH_2	29.9912	14	13	3	0	8	2422	2721	2615	2885	3116						
17	C <sup>13</sup> CH_5	30.0428	3832	3832	3364	2693	2471	4699	5130	4936	5133	5389						
18	<sup>30</sup> SiH	30.9801	8	13	6	1	4	2173	2422	2217	2518	2809						
19	SiH_3	31.0003	21	18	5	3	6	3507	3781	3553	3876	4465						
20	CH_3O	31.019	1333	1354	1226	945	832	3155	3377	3407	3465	3673						
21	CH_2Na	37.0056	430	480	399	300	324	621	739	754	712	746						
22	CH_3Na	38.0139	2984	3010	2527	1970	1925	4109	4382	4349	4737	4682						
23	K	38.9643	8092	8715	10122	8387	6862	53753	60170	70205	71900	74700						
24	C_3H_3	39.0223	65100	66159	56944	45688	43858	74688	76288	73788	73488	77249						
25	Ca	39.9603	97	84	63							1307						
26	C_3H_4	40.0303	8344	8715	7588													
27	C_2HO	41.002	12230	13196	10909													
28	C_3H_5	41.0386	217861	218907	190576													
29	Unknown	41.99	107	102	81													
30	C_2H_2O	42.0105	1544	1518	1278													
31	C_3H_6	42.0457	39557	38921	35316	2743												
32	SiCH3	42.9991	158	137	127													
33	C_2H_3O	43.0192	4696	4543	4135	3106	2897	6183	6294	6407	6591	5173						
34	C_3H_7	43.055	248655	247109	219552	184767	174484	300864	319759	326088	318696	335491						
35	<sup>29</sup> SiCH_3	43.9983	6	11	11	5	7	624	698	715	788	786						
36	SiCH4	44.0069	10	18	10	12	9	1218	1373	1218	1401	1637						
37	C_2H_4O	44.0254	440	424	384	286	282	846	889	956	932	995						
38	C_2 <sup>13</sup> CH	44.0585	10401	10490	9619	7498	7052	13826	14572	15011	15023	15600						
39	SiHO	44.9792	31	20	9	10	18	2907	3019	2837	3080	3657						
40	CHO_2	44.9965	133	131	106	72	73	836	936	924	955	1020						
41	SiCH_5	45.0157	52	49	36	21	24	4907	5275	5059	5635	6272						
42	C_2H_5O	45.035	1616	1653	1572	1148	1037	3358	3606	3639	3762	3843						
43	SiH_3O	46.9949	13	6	6	4	3	402	390	369	404	461						
44	CH_3O_2	47.0119	95	95	69	75	62	393	480	420	498	539						
45	C_4H_2	50.0137	883	925	720	561	537	1328	1522	1474	1629	1649						

If these dialogs appear, choose 'OK' to save only the active sheet.

contain multiple sheets.

- To save only the active sheet, click OK.
- To save all sheets, save them individually using different file name for each, or choose a file type that supports multiple sheets.

OK Cancel



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	Ion	Mass	MOC01_0	MOC01_02	MOC01_03	MOC01_04	MOC01_05	MOC03_0	MOC03_02	MOC03_03	MOC03_04	MOC03_05						
2	CH	13.0075	649	727	600	450	429	827	957	973	962	955						
3	CH_2	14.0154	3637	3652	2921	2336	2005	4365	4846	4763	5043	4785						
4	CH_3	15.0235	16798	17225	14481	11674	10776	20996	22684	22824	23978	23233						
5	H_3O	19.0189	421	417	343	331	237	968	1029	1024	1008	1088						
6	Na	22.9906	114	59	49	26	38	1399	1243	1170	1149	1364						
7	C_2H_2	26.0149	8921	9309	8001	6199	5973	11350	12875	12634	12730	13103						
8	Al	26.9807	30	26	19	11	12	2387	2514	2661	2506	3088						
9	C_2H_3	27.0234	160972	163472	143259	114190	110734	199721	214426	215485	217814	227691						
10	Si	27.9756	317	219	157	14	106	56397	61199	57741	63527	70902						
11	C_2H_4	28.031	13982	14213	12345	9510	8912	15944	17155	17316	17141	17879						
12	SiH	28.9833	305	293	167	23	108	57119	63742	60168	65080	72225						
13	C_2H_5	29.0393	154411	153973	136133	110304	104090	157226	166928	170664	163458	168904						
14	<sup>30</sup> Si	29.9722	14	11	5	0	4	1818	2116	1908	2131	2322						
15	<sup>29</sup> SiH	29.9828	14	14	11	2	4	3001	3429	3184	3416	3831						
16	SiH_2	29.9912	14	13	3	0	8	2422	2721	2615	2885	3116						
17	C <sup>13</sup> CH_5	30.0428	3832	3832	3364	2693	2471	4699	5130	4936	5133	5389						
18	<sup>30</sup> SiH	30.9801	8	13	6	1	4	2173	2422	2217	2518	2809						
19	SiH_3	31.0003	21	18	5	3	6	3507	3781	3553	3876	4465						
20	CH_3O	31.019	1333	1354	1226	945	832	3155	3377	3407	3465	3673						
21	CH_2Na	37.0056	430	480	399	300	324	621	739	754	712	746						
22	CH_3Na	38.0139	2984	3010	2527	1970	1925	4109	4382	4349	4737	4682						
23	K	38.9643	8092	8715	10122	8387	6862	53753	60170	70205	71900	74700						
24	C_3H_3	39.0223	65100	66159	569						8162	77249						
25	Ca	39.9603	97	84							443	1307						
26	C_3H_4	40.0303	8344	8715	75													
27	C_2HO	41.002	12230	13196	109													
28	C_3H_5	41.0386	217861	218907	190													
29	Unknown	41.99	107	102	81													
30	C_2H_2O	42.0105	1544	1518	1278													
31	C_3H_6	42.0457	39557	38921	35316	27												
32	SiCH3	42.9991	158	137	127													
33	C_2H_3O	43.0192	4696	4543	4135	3												
34	C_3H_7	43.055	248655	247109	219552	184767	174484	300864	319759	326088	318696	335491						
35	<sup>29</sup> SiCH_3	43.9983	6	11	11	5	7	624	698	715	788	786						
36	SiCH4	44.0069	10	18	10	12	9	1218	1373	1218	1401	1637						
37	C_2H_4O	44.0254	440	424	384	286	282	846	889	956	932	995						
38	C_2 <sup>13</sup> CH	44.0585	10401	10490	9619	7498	7052	13826	14572	15011	15023	15600						
39	SiHO	44.9792	31	20	9	10	18	2907	3019	2837	3080	3657						
40	CHO_2	44.9965	133	131	106	72	73	836	936	924	955	1020						
41	SiCH_5	45.0157	52	49	36	21	24	4907	5275	5059	5635	6272						
42	C_2H_5O	45.035	1616	1653	1572	1148	1037	3358	3606	3639	3762	3843						
43	SiH_3O	46.9949	13	6	6	4	3	402	390	369	404	461						
44	CH_3O_2	47.0119	95	95	69	75	62	393	480	420	498	539						
45	C_4H_2	50.0137	883	925	720	561	537	1328	1522	1474	1629	1649						

Choose 'Yes' to keep the current format.

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 copy in the latest Excel format.
- To see what might be lost, click Help.

Yes No Help

Microsoft Excel - fortutorial.txt

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Microsoft Word Ribbon: Font (Arial, 10, Bold), Paragraph, Styles, Tables, References, Send To Mobile, Window, Help

Close the file.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	Ion	Mass	MOC01_0	MOC01_02	MOC01_03	MOC01_04	MOC01_05	MOC03_0	MOC03_02	MOC03_03	MOC03_04	MOC03_05	MOC03_06	MOC03_07	MOC03_08	MOC03_09	MOC03_10	MOC03_11
2	CH	13.0075	649	727	600	450	429	827	957	973	962	955						
3	CH_2	14.0154	3637	3652	2921	2336	2005	4365	4846	4763	5043	4785						
4	CH_3	15.0235	16798	17225	14481	11674	10776	20996	22684	22824	23978	23233						
5	H_3O	19.0189	421	417	343	331	237	968	1029	1024	1008	1088						
6	Na	22.9906	114	59	49	26	38	1399	1243	1170	1149	1364						
7	C_2H_2	26.0149	8921	9309	8001	6199	5973	11350	12875	12634	12730	13103						
8	Al	26.9807	30	26	19	11	12	2387	2514	2661	2506	3088						
9	C_2H_3	27.0234	160972	163472	143259	114190	110734	199721	214426	215485	217814	227691						
10	Si	27.9756	317	219	157	14	106	56397	61199	57741	63527	70902						
11	C_2H_4	28.031	13982	14213	12345	9510	8912	15944	17155	17316	17141	17879						
12	SiH	28.9833	305	293	167	23	108	57119	63742	60168	65080	72225						
13	C_2H_5	29.0393	154411	153973	136133	110304	104090	157226	166928	170664	163458	168904						
14	<sup>30</sup> Si	29.9722	14	11	5	0	4	1818	2116	1908	2131	2322						
15	<sup>29</sup> SiH	29.9828	14	14	11	2	4	3001	3429	3184	3416	3831						
16	SiH_2	29.9912	14	13	3	0	8	2422	2721	2615	2885	3116						
17	C <sup>13</sup> CH_5	30.0428	3832	3832	3364	2693	2471	4699	5130	4936	5133	5389						
18	<sup>30</sup> SiH	30.9801	8	13	6	1	4	2173	2422	2217	2518	2809						
19	SiH_3	31.0003	21	18	5	3	6	3507	3781	3553	3876	4465						
20	CH_3O	31.019	1333	1354	1226	945	832	3155	3377	3407	3465	3673						
21	CH_2Na	37.0056	430	480	399	300	324	621	739	754	712	746						
22	CH_3Na	38.0139	2984	3010	2527	1970	1925	4109	4382	4349	4737	4682						
23	K	38.9643	8092	8715	10122	8387	6862	53753	60170	70205	71900	74700						
24	C_3H_3	39.0223	65100	66159	56944	45668	43959	71666	76298	72796	73162	77249						
25	Ca	39.9603	97	84	63	37	63	1407	1584	1299	1443	1307						
26	C_3H_4	40.0303	8344	8715	7588	5847	5497	11982	12709	12615	13108	13817						
27	C_2HO	41.002	12230	13196	10909	9437	8351	16219	18235	17269	18981	18934						
28	C_3H_5	41.0386	217861	218907	190576	160395	151292	275246	291714	291195	293492	305962						
29	Unknown	41.99	107	102	81	63	54	4492	5032	4468	5224	5744						
30	C_2H_2O	42.0105	1544	1518	1278	957	821	2295	2370	2473	2402	2631						
31	C_3H_6	42.0457	39557	38921	35316	27436	25695	49622	51063	52611	53047	55709						
32	SiCH3	42.9991	158	137	127	80	93	13253	14304	13448	15217	16708						
33	C_2H_3O	43.0192	4696	4543	4135	3106	2897	8105	8294	8467	8531	9173						
34	C_3H_7	43.055	248655	247109	219552	184767	174484	300864	319759	326088	318696	335491						
35	<sup>29</sup> SiCH_3	43.9983	6	11	11	5	7	624	698	715	788	786						
36	SiCH4	44.0069	10	18	10	12	9	1218	1373	1218	1401	1637						
37	C_2H_4O	44.0254	440	424	384	286	282	846	889	956	932	995						
38	C_2 <sup>13</sup> CH	44.0585	10401	10490	9619	7498	7052	13826	14572	15011	15023	15600						
39	SiHO	44.9792	31	20	9	10	18	2907	3019	2837	3080	3657						
40	CHO_2	44.9965	133	131	106	72	73	836	936	924	955	1020						
41	SiCH_5	45.0157	52	49	36	21	24	4907	5275	5059	5635	6272						
42	C_2H_5O	45.035	1616	1653	1572	1148	1037	3358	3606	3639	3762	3843						
43	SiH_3O	46.9949	13	6	6	4	3	402	390	369	404	461						
44	CH_3O_2	47.0119	95	95	69	75	62	393	480	420	498	539						
45	C_4H_2	50.0137	883	925	720	561	537	1328	1522	1474	1629	1649						

fortutorial / Sheet2 / Sheet3

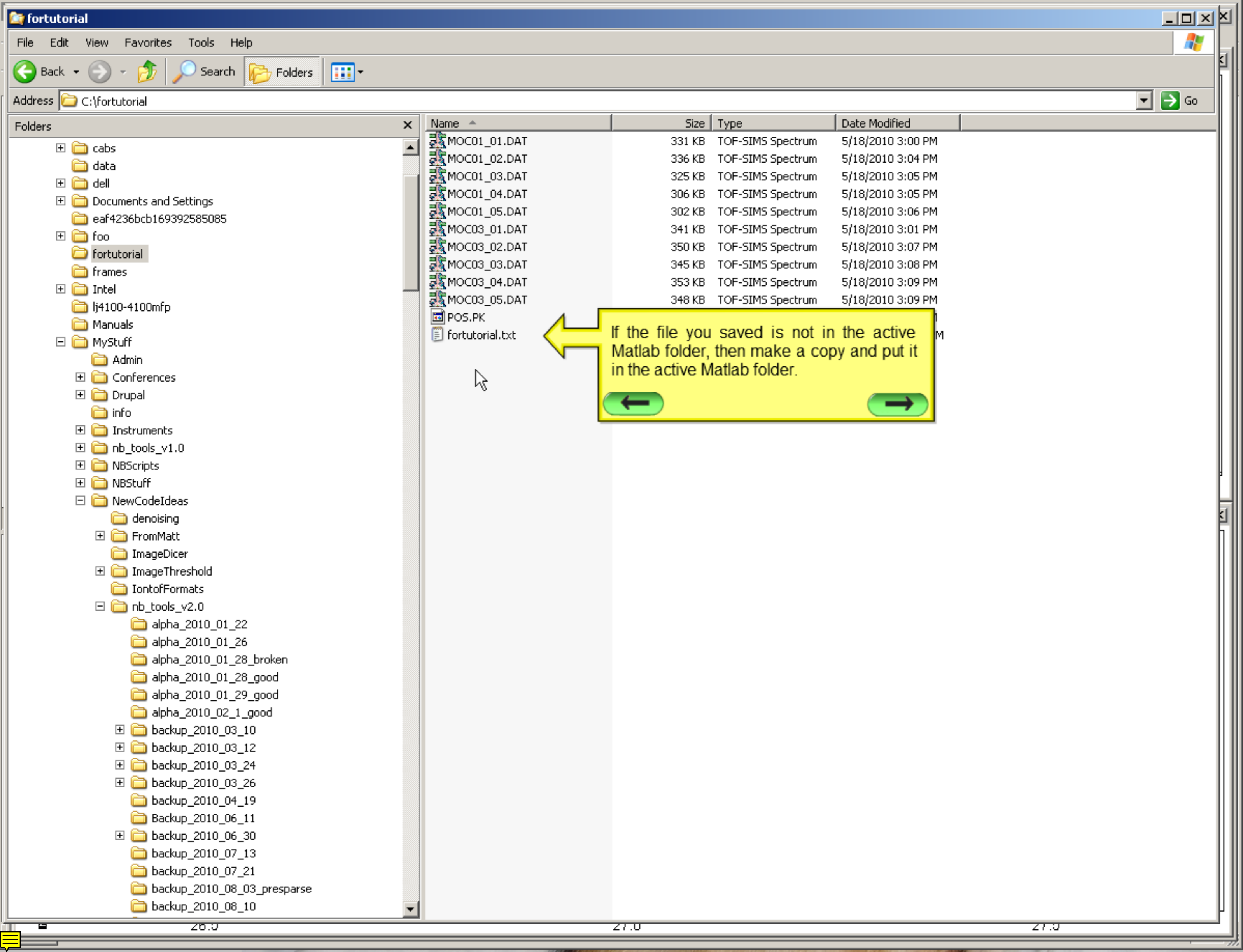
Ready NUM

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	Ion	Mass	MOC01_0	MOC01_0	MOC01_0	MOC01_0	MOC01_0	MOC03_0	MOC03_0	MOC03_0	MOC03_0	MOC03_0						
2	CH	13.0075	649	727	600	450	429	827	957	973	962	955						
3	CH_2	14.0154	3637	3652	2921	2336	2005	4365	4846	4763	5043	4785						
4	CH_3	15.0235	16798	17225	14481	11674	10776	20996	22684	22824	23978	23233						
5	H_3O	19.0189	421	417	343	331	237	968	1029	1024	1008	1088						
6	Na	22.9906	114	59	49	26	38	1399	1243	1170	1149	1364						
7	C_2H_2	26.0149	8921	9309	8001	6199	5973	11350	12875	12634	12730	13103						
8	Al	26.9807	30	26	19	11	12	2387	2514	2661	2506	3088						
9	C_2H_3	27.0234	160972	163472	143259	114190	110734	199721	214426	215485	217814	227691						
10	Si	27.9756	317	219	157	14	106	56397	61199	57741	63527	70902						
11	C_2H_4	28.031	13982	14213	12345	9510	8912	15944	17155	17316	17141	17879						
12	SiH	28.9833	305	293	167	23	108	57119	63742	60168	65080	72225						
13	C_2H_5	29.0393	154411	153973	136133	110304	104090	157226	166928	170664	163458	168904						
14	<sup>30</sup> Si	29.9722	14	11	5	0	4	1818	2116	1908	2131	2322						
15	<sup>29</sup> SiH	29.9828	14	14	11	2	4	3001	3429	3184	3416	3831						
16	SiH_2	29.9912	14	13	3	0	8	2422	2721	2615	2885	3116						
17	C <sup>13</sup> CH_5	30.0428	3832	3832	3364	2693	2471	4699	5130	4936	5133	5389						
18	<sup>30</sup> SiH	30.9801	8	13	6	1	4	2173	2422	2217	2518	2809						
19	SiH_3	31.0003	21	18	5	3	6	3507	3781	3553	3876	4465						
20	CH_3O	31.019	1333	1354	1226	945	832	3155	3377	3407	3465	3673						
21	CH_2Na	37.0056	430	480	399	300	324	621	739	754	712	746						
22	CH_3Na	38.0139	2984	3010	2527	1970	1925	4109	4382	4349	4737	4682						
23	K	38.9643	8092	8715	10122	838												
24	C_3H_3	39.0223	65100	66159	56944	4566												
25	Ca	39.9603	97	84	63	3												
26	C_3H_4	40.0303	8344	8715	7588	584												
27	C_2HO	41.002	12230	13196	10909	943												
28	C_3H_5	41.0386	217861	218907	190576	16039												
29	Unknown	41.99	107	102	81	63	54	4492										
30	C_2H_2O	42.0105	1544	1518	1278	957	821	2295										
31	C_3H_6	42.0457	39557	38921	35316	27436	25695	49622										
32	SiCH3	42.9991	158	137	127	80	93	13253										
33	C_2H_3O	43.0192	4696	4543	4135	3106	2897	8105	8294	8467	8531	9173						
34	C_3H_7	43.055	248655	247109	219552	184767	174484	300864	319759	326088	318696	335491						
35	<sup>29</sup> SiCH_3	43.9983	6	11	11	5	7	624	698	715	788	786						
36	SiCH4	44.0069	10	18	10	12	9	1218	1373	1218	1401	1637						
37	C_2H_4O	44.0254	440	424	384	286	282	846	889	956	932	995						
38	C_2 <sup>13</sup> CH	44.0585	10401	10490	9619	7498	7052	13826	14572	15011	15023	15600						
39	SiHO	44.9792	31	20	9	10	18	2907	3019	2837	3080	3657						
40	CHO_2	44.9965	133	131	106	72	73	836	936	924	955	1020						
41	SiCH_5	45.0157	52	49	36	21	24	4907	5275	5059	5635	6272						
42	C_2H_5O	45.035	1616	1653	1572	1148	1037	3358	3606	3639	3762	3843						
43	SiH_3O	46.9949	13	6	6	4	3	402	390	369	404	461						
44	CH_3O_2	47.0119	95	95	69	75	62	393	480	420	498	539						
45	C_4H_2	50.0137	883	925	720	561	537	1328	1522	1474	1629	1649						

Choose 'No' if it asks if you want to save changes. We already saved what we needed.

Do you want to save the changes you made to 'fortutorial.txt'?

Yes No Cancel



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  - [-] Admin
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  - [-] Drupal
  - [-] info
  - [-] Instruments
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  - [-] NBScripts
  - [-] NBStuff
  - [-] NewCodeIdeas
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    - [-] ImageThreshold
    - [-] IontofFormats
    - [-] nb\_tools\_v2.0
      - alpha\_2010\_01\_22
      - alpha\_2010\_01\_26
      - alpha\_2010\_01\_28\_broken
      - alpha\_2010\_01\_28\_good
      - alpha\_2010\_01\_29\_good
      - alpha\_2010\_02\_1\_good
  - [-] backup\_2010\_03\_10
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  - [-] backup\_2010\_08\_03\_presparse
  - [-] backup\_2010\_08\_10

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MOC01_02.DAT	336 KB	TOF-SIMS Spectrum	5/18/2010 3:04 PM
MOC01_03.DAT	325 KB	TOF-SIMS Spectrum	5/18/2010 3:05 PM
MOC01_04.DAT	306 KB	TOF-SIMS Spectrum	5/18/2010 3:05 PM
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MOC03_01.DAT	341 KB	TOF-SIMS Spectrum	5/18/2010 3:01 PM
MOC03_02.DAT	350 KB	TOF-SIMS Spectrum	5/18/2010 3:07 PM
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POS.PK			
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- Movie Maker
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S1GL_05.BIF	10,114 KB	BIF File	9/9/2010 3:43 PM
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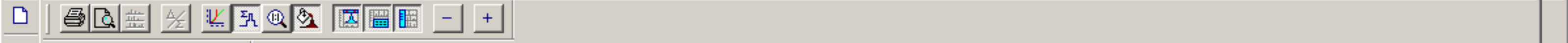
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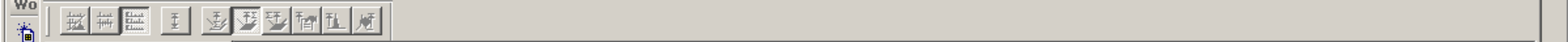






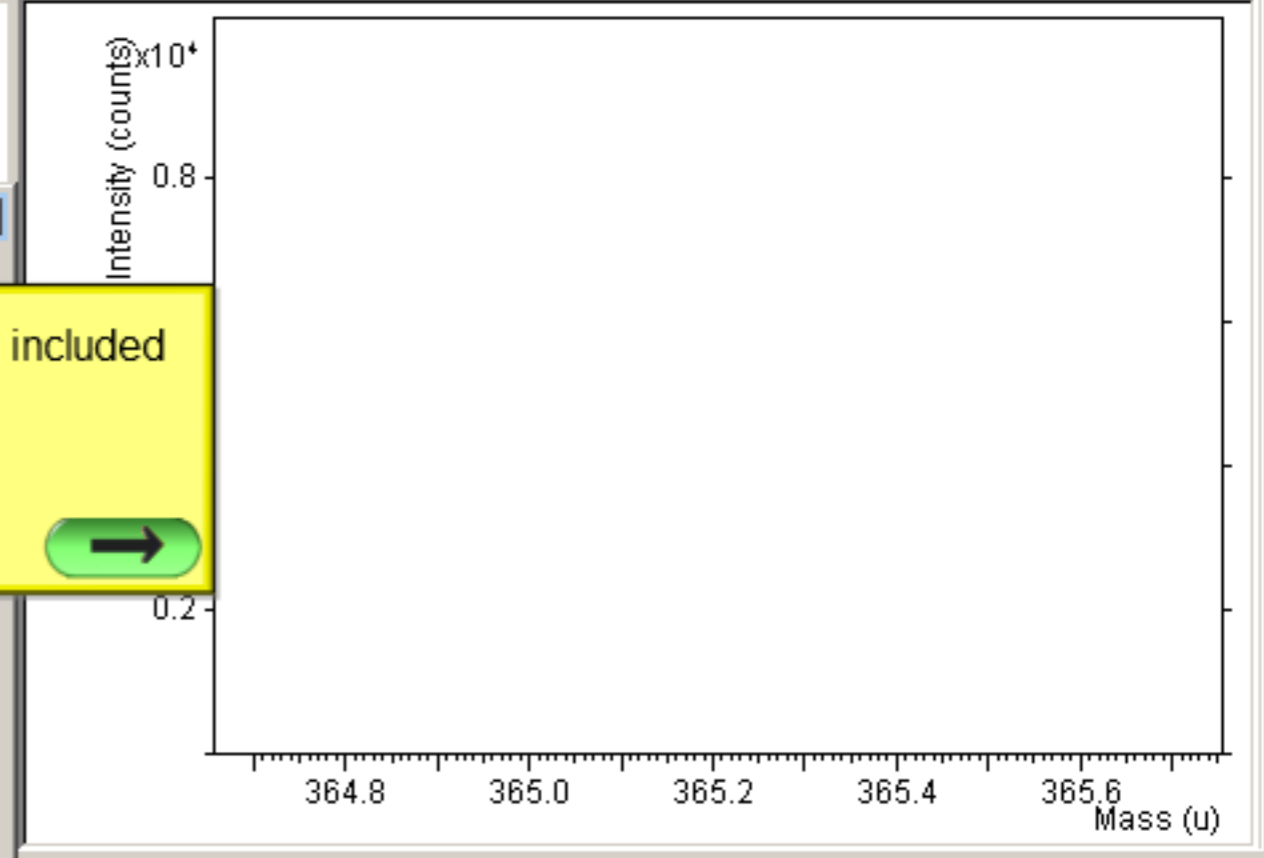


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Compilations Spectrum Properties

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	Check...	Add Peak	Dev. (ppm)	<input type="text"/>	Peak Difference...	Poisson Corr. (%)	<input type="text"/>	Error (%)	0.0	Width (ns)	<input type="text"/>



Spectra Finder (TOF-SIMS)

C:\fortutorial

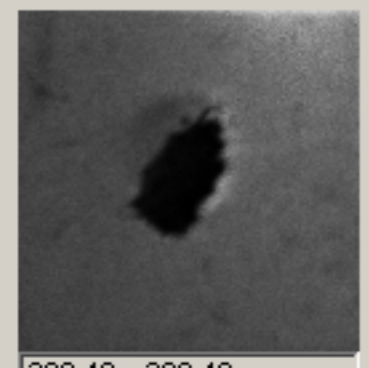
- 1100\_01\_1.ITS
- 1100\_02\_ITS
- 1100\_06\_ITS
- 5100\_01\_ITS
- 5100\_06\_ITS
- 25100\_01\_ITS
- 25500\_01\_ITS
- 51000\_01\_ITS

Select all the files you want to be included in your peak area table.

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Sample:

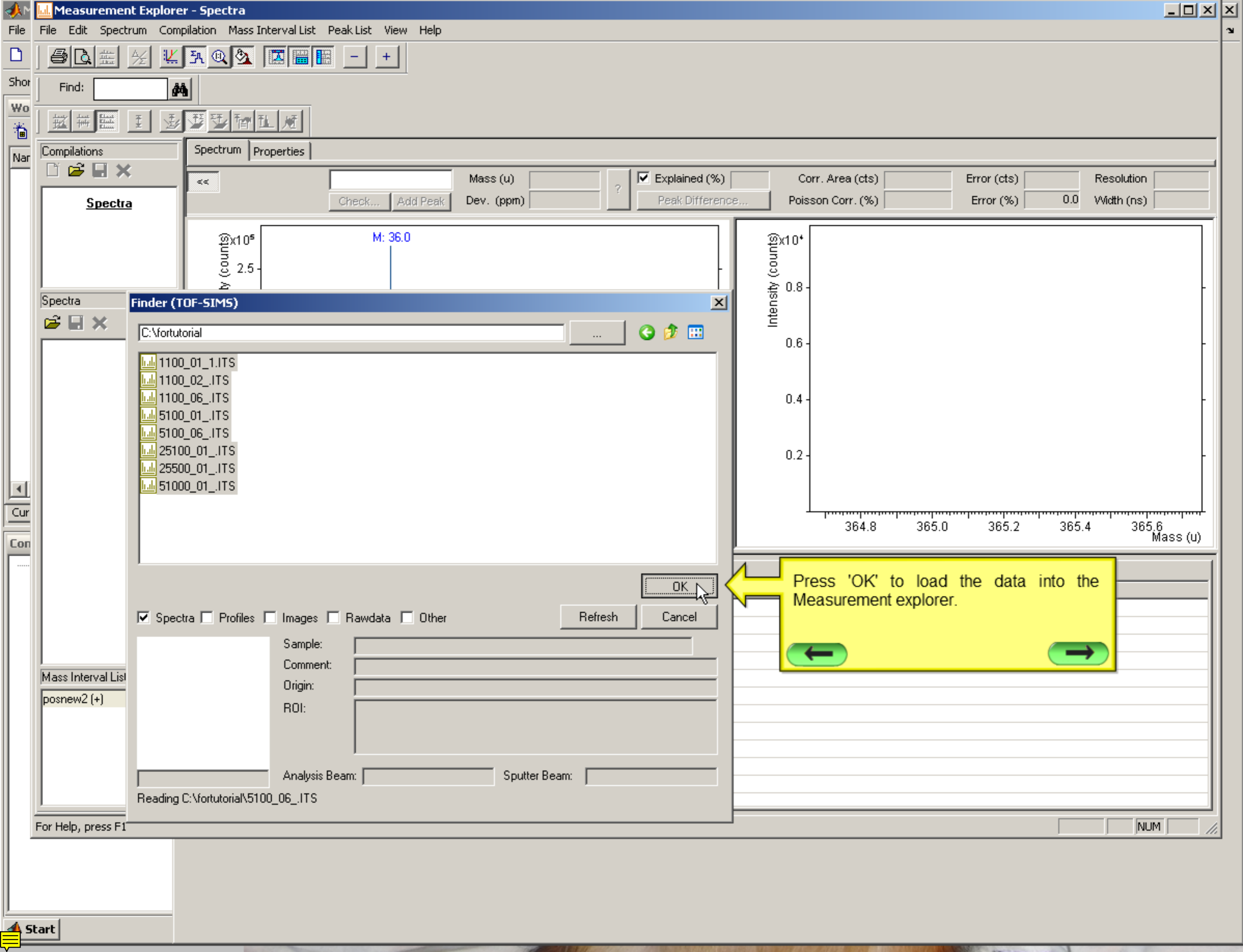
Comment:

Origin:

ROI: z-ROI: start scan 1, stop scan 25, total scans 25

399.40 x 399.40 μm Analysis Beam:  Sputter Beam:

Reading C:\fortutorial\5100\_06\_ITS



**Finder (TOF-SIMS)**

C:\fortutorial

- 1100\_01\_1.ITS
- 1100\_02\_ITS
- 1100\_06\_ITS
- 5100\_01\_ITS
- 5100\_06\_ITS
- 25100\_01\_ITS
- 25500\_01\_ITS
- 51000\_01\_ITS

Spectra  Profiles  Images  Rawdata  Other

Sample: \_\_\_\_\_  
Comment: \_\_\_\_\_  
Origin: \_\_\_\_\_  
ROI: \_\_\_\_\_

Analysis Beam: \_\_\_\_\_ Sputter Beam: \_\_\_\_\_

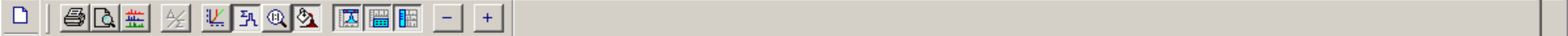
Reading C:\fortutorial\5100\_06\_ITS

OK Refresh Cancel

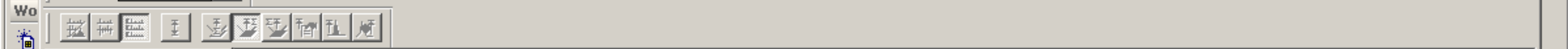
Press 'OK' to load the data into the Measurement explorer.







Find:



Compilations

Spectra

1100\_01\_1  
1100\_02\_  
1100\_06\_  
5100\_01\_  
5100\_06\_  
25100\_01\_  
25500\_01\_  
**51000\_01**

Mass Interval Lists

posnew2 (+)

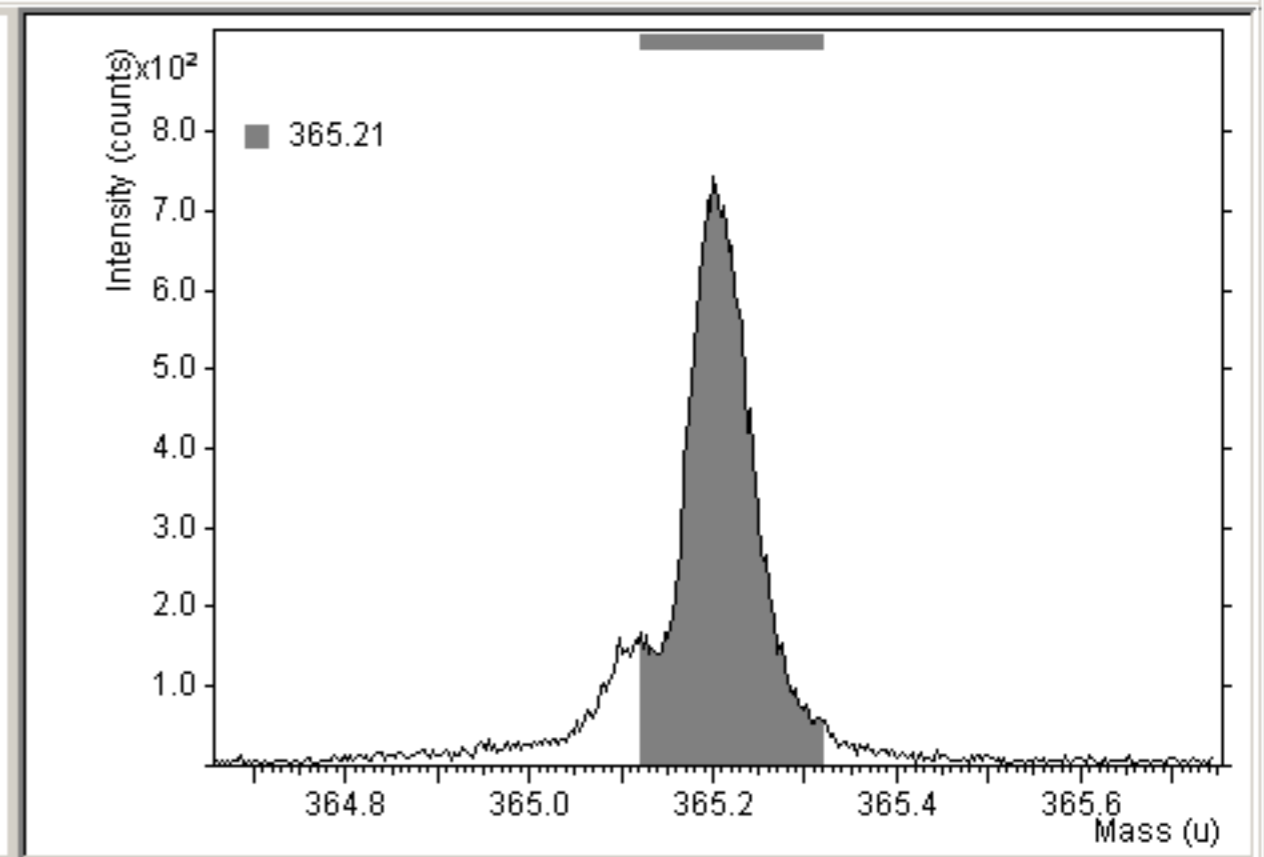
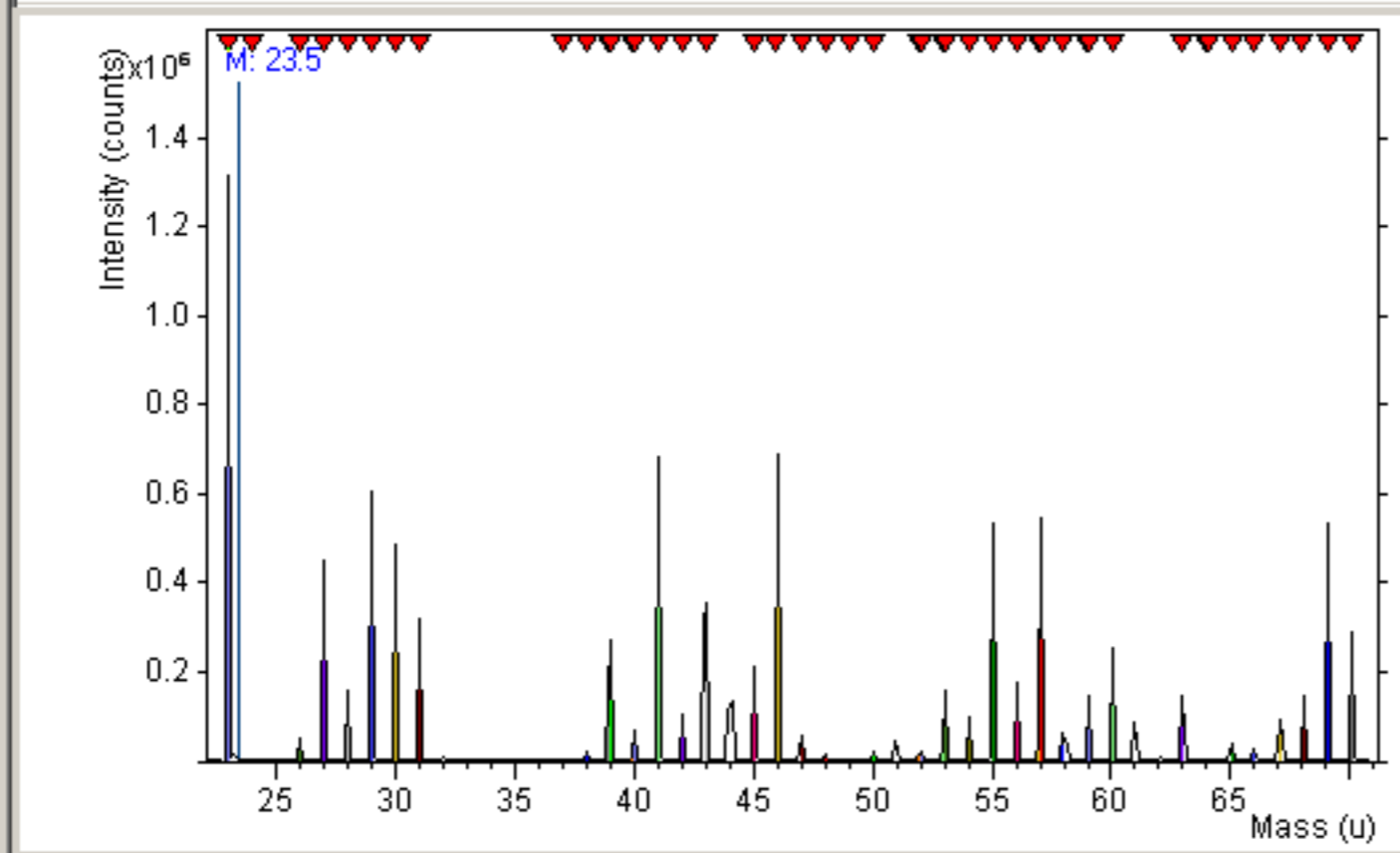
Statistic

Spectrum Properties

CH\_30Be+ Mass (u) 40.0302 Explained (%) 100.0 Corr. Area (cts) 60,498 Error (cts) 248 Resolution 5,302

Dev. (ppm) 5.1 Peak Difference... Poisson Corr. (%) 1.9 Error (%) 0.0 Width (ns) 2.06

Check... Add Peak



✓	No.	Center Mas...	Corrected Ar...	Color	Peak Label
✓	1	15.0236	143045	Red	
✓	2	15.9940	4318	Blue	
✓	3	17.0019	1022	Green	
✓	4	17.0262	3670	Grey	
✓	5	18.0352	42711	Orange	
✓	6	22.9913	2793823	Light Blue	
✓	7	23.9843	2002	Light Green	
✓	8	26.0148	48788	Dark Green	
✓	9	27.0233	504621	Purple	
✓	10	28.0187	66699	Olive	
✓	11	28.0312	74139	Light Grey	
✓	12	29.0028	300321	Green	

Once the peaks show up in this box, push the 'Statistic' button

Find:

Workbench icons:

Compilations

Spectra

- 1100\_01\_
- 1100\_02\_
- 1100\_06\_
- 5100\_01\_
- 5100\_06\_
- 25100\_01\_
- 25500\_01\_
- 51000\_01\_**

Mass Interval Lists

posnew2 (+)

Spectrum Properties

CH\_30Be+ Mass (u) 40.0302 ? Explained (%) 100.0 Corr. Area (cts) 60,498 Error (cts) 248 Resolution 5,302

Dev. (ppm) 5.1 Peak Difference... Poisson Corr. (%) 1.9 Error (%) 0.0 Width (ns) 2.06

Peak Statistics

Ion	Mass	1100_01_1	1100_02_	1100_06_	5100_01_	5100_06_	25100_01_	25500_01_	51000_01_
	15.0236	33461.3800	140278.4831	195.0116	138903.1592	143.0062	149607.3044	142110.7742	143044.6
	15.9940	33.0003	7493.1085	648218.3548	7510.1865	539516.0194	7760.3496	7785.4685	4317.6
	17.0019	4.0000	1634.8153	286086.8354	1589.7710	238737.7805	1637.8183	1602.7837	1022.0
	17.0262	66.0013	1264.4878	97.0029	1470.6598	79.0019	1491.6788	1469.6590	3670.0
	18.0352	6504.8960	21063.82				510.6716	27598.1397	42710.0
	22.9913	455978.5309	20				615.7764	2934920.8630	2793823.0
	23.9843	542.0897					800.2188	4710.7658	2002.0
	26.0148	3155.0358	52026.35				838.7328	52428.9901	48788.0
	27.0233	76671.3134	536084.95				138.1868	520893.5693	504620.0
	28.0187	5831.3651	24001.95				192.4718	25907.7623	66699.0
	28.0312	14540.3302	68572.16				905.0137	69490.0376	74139.0
	29.0028	65847.6662	364989.75				122.8091	349239.0902	300321.0
	29.0399	186753.4311	374481.18				1047.7362	357022.1301	346403.0
	29.9981	24515.5023	495818.9592	7733.2217	476549.2521	6426.5876	518144.5731	490149.8896	405782.0
	30.0355	13315.9659	34928.6867	8.0000	29409.3778	8.0000	29951.1030	36942.3725	96829.0
	31.0189	88250.6581	412657.8088	1005.3084	374779.0682	813.2018	413271.5480	389597.0510	339247.0
	37.0060	472.0680	4720.7946	1001.3059	5127.0136	743.1685	5350.7278	4942.4473	4401.0
	38.0143	1106.3735	20372.1319	889.2413	20081.5668	710.1539	21680.8196	20082.5791	20827.0
	38.9655	28284.7500	65280.4146	1.0000	54068.4155	1.0000	64290.0167	99202.5726	84705.0
	39.0227	52279.2818	320261.4895	606.1121	328864.5364	398.0483	352194.6225	298491.6540	286046.0
	39.9605	794.1925	42016.1687	0.0000	38310.4324	0.0000	40879.7812	18564.7830	9275.0
	40.0304	13284.7132	56705.0582	826.2083	54005.3701	537.0880	59937.0824	54675.2225	56746.0
	41.0394	258207.3606	866719.0906	890.2418	839310.0869	508.0788	949671.0793	796298.2218	700251.0
	42.0103	20659.7105	77005.6303	21105.3545	71163.3428	15147.8091	76636.7327	73606.9521	70709.0

This table is automatically calculated and populated.

Make sure the following settings are used.

← →

<input checked="" type="checkbox"/>	6	22.9913	2793823		
<input checked="" type="checkbox"/>	7	23.9843	2002		
<input checked="" type="checkbox"/>	8	26.0148	48788		
<input checked="" type="checkbox"/>	9	27.0233	504621		
<input checked="" type="checkbox"/>	10	28.0187	66699		
<input checked="" type="checkbox"/>	11	28.0312	74139		
<input checked="" type="checkbox"/>	12	29.0028	300321		

Find:

Compilations

Spectra

CH\_30Be+ Mass (u) 40.0302 ? Explained (%) 100.0 Corr. Area (cts) 60,498 Error (cts) 248 Resolution 5,302

Check... Add Peak Dev. (ppm) 5.1 Peak Difference... Poisson Corr. (%) 1.9 Error (%) 0.0 Width (ns) 2.06

Spectra

1100\_01\_1

1100\_02\_

1100\_06\_

5100\_01\_

5100\_06\_

25100\_01\_

25500\_01\_

51000\_01

Peak Statistics

Ion	Mass	1100_01_1	1100_02_	1100_06_	5100_01_	5100_06_	25100_01_	25500_01_	51000_01_
	15.0236	33461.3800	140278.4831	195.0116	138903.1592	143.0062	149607.3044	142110.7742	143044.6
	15.9940	33.0003	7493.1085	648218.3548	7510.1865	539516.0194	7760.3496	7785.4685	4317.6
	17.0019	4.0000	1634.8153	286086.8354	1589.7710	238737.7805	1637.8183	1602.7837	1022.0
	17.0262	66.0013	1264.4878	97.0029	1470.6598	79.0019	1491.6788	1469.6590	3670.0
	18.0352	6504.8960				0.0000	43510.6716	27598.1397	42710.0
	22.9913	455978.5309	2			26.0002	2120615.7764	2934920.8630	2793823.0
	23.9843	542.0897				714.1556	15300.2188	4710.7658	2002.0
	26.0148	3155.0358				10206.0186	53228.7228	52428.0001	48788.0
	27.0233	76671.3134							
	28.0187	5831.3651							
	28.0312	14540.3302							
	29.0028	65847.6662							
	29.0399	186753.4311							
	29.9981	24515.5023							
	30.0355	13315.9659							
	31.0189	88250.6581							
	37.0060	472.0680	4720.7946	1001.3059	5127.0136	743.1685	5350.7278	4942.4473	4401.0
	38.0143	1106.3735	20372.1319	889.2413	20081.5668	710.1539	21680.8196	20082.5791	20827.0
	38.9655	28284.7500	65280.4146	1.0000	54068.4155	1.0000	64290.0167	99202.5726	84705.0
	39.0227	52279.2818	320261.4895	606.1121	328864.5364	398.0483	352194.6225	298491.6540	286046.0
	39.9605	794.1925	42016.1687	0.0000	38310.4324	0.0000	40879.7812	18564.7830	9275.0
	40.0304	13284.7132	56705.0582	826.2083	54005.3701	537.0880	59937.0824	54675.2225	56746.0
	41.0394	258207.3606	866719.0906	890.2418	839310.0869	508.0788	949671.0793	796298.2218	700251.0
	42.0103	20659.7105	77005.6303	21105.3545	71163.3428	15147.8091	76636.7327	73606.9521	70709.0

Statistic Data List Layout Option

Print Precision:

Mass:

Others:

Cancel OK

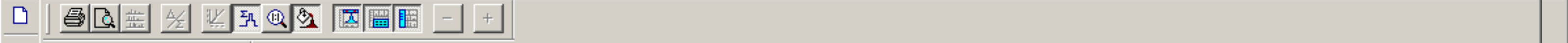
Check the print precision. I typically use 4 and 4.

← →

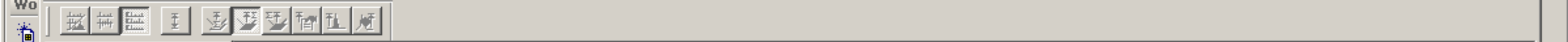
Mass Interval Lists

posnew2 (+)

<input checked="" type="checkbox"/>	6	22.9913	2793823	
<input checked="" type="checkbox"/>	7	23.9843	2002	
<input checked="" type="checkbox"/>	8	26.0148	48788	
<input checked="" type="checkbox"/>	9	27.0233	504621	
<input checked="" type="checkbox"/>	10	28.0187	66699	
<input checked="" type="checkbox"/>	11	28.0312	74139	
<input checked="" type="checkbox"/>	12	29.0028	300321	



Find:



Compilations

Spectra

CH\_30Be+ Mass (u) 40.0302 ?  Explained (%) 100.0 Corr. Area (cts) 60,498 Error (cts) 248 Resolution 5,302

Check... Add Peak Dev. (ppm) 5.1 ? Peak Difference... Poisson Corr. (%) 1.9 Error (%) 0.0 Width (ns) 2.06

Peak Statistics

The 'List by column' button should be selected.

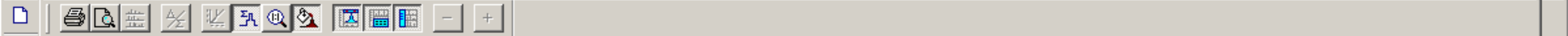
Ion	5100_01	5100_06	25100_01	25500_01	51000_01
16	138903.1592	143.0062	149607.3044	142110.7742	143044.6
48	7510.1865	539516.0194	7760.3496	7785.4685	4317.6
54	1589.7710	238737.7805	1637.8183	1602.7837	1022.0
29	1470.6598	79.0019	1491.6788	1469.6590	3670.0
18.0352	6504.8960	21063.8234	1.0000	37557.1931	0.0000
22.9913	455978.5309	2084823.5888	40.0005	2032262.6821	26.0002
23.9843	542.0897	14301.2350	743.1685	15212.4049	714.1556
26.0148	3155.0358	52026.3577	13261.5262	53688.1127	10396.9186
27.0233	76671.3134	536084.9564	908.2517	535729.9026	582.1034
28.0187	5831.3651	24001.9545	92.0026	21611.9153	65.0013
28.0312	14540.3302	68572.1682	64.0013	66197.4825	48.0007
29.0028	65847.6662	364989.7575	1760.9460	336658.0049	1187.4302
29.0399	186753.4311	374481.1806	8.0000	367438.1770	4.0000
29.9981	24515.5023	495818.9592	7733.2217	476549.2521	6426.5876
30.0355	13315.9659	34928.6867	8.0000	29409.3778	8.0000
31.0189	88250.6581	412657.8088	1005.3084	374779.0682	813.2018
37.0060	472.0680	4720.7946	1001.3059	5127.0136	743.1685
38.0143	1106.3735	20372.1319	889.2413	20081.5668	710.1539
38.9655	28284.7500	65280.4146	1.0000	54068.4155	1.0000
39.0227	52279.2818	320261.4895	606.1121	328864.5364	398.0483
39.9605	794.1925	42016.1687	0.0000	38310.4324	0.0000
40.0304	13284.7132	56705.0582	826.2083	54005.3701	537.0880
41.0394	258207.3606	866719.0906	890.2418	839310.0869	508.0788
42.0103	20659.7105	77005.6303	21105.3545	71163.3428	15147.8091

Mass Interval Lists

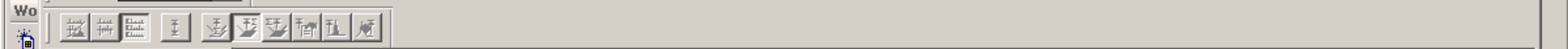
posnew2 (+)

Ion	Mass (u)	Area (cts)	Color
6	22.9913	2793823	Blue
7	23.9843	2002	Green
8	26.0148	48788	Dark Green
9	27.0233	504621	Purple
10	28.0187	66699	Olive
11	28.0312	74139	Grey
12	29.0028	300321	Light Green





Find:



Compilations

Spectra

CH\_30Be+ Mass (u) 40.0302 ?  Explained (%) 100.0 Corr. Area (cts) 60,498 Error (cts) 248 Resolution 5,302

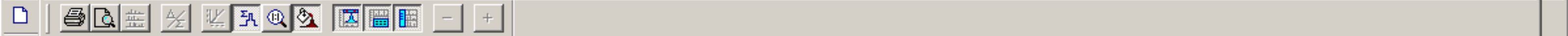
Check... Add Peak Dev. (ppm) 5.1 ? Peak Difference... Poisson Corr. (%) 1.9 Error (%) 0.0 Width (ns) 2.06

Peak Statistics

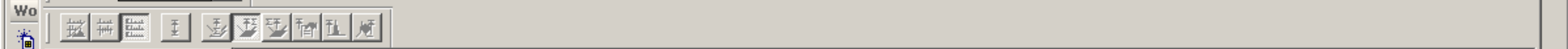
The 'List spectrum data' button should be selected.

Ion	5100_01_	5100_06_	25100_01_	25500_01_	51000_01_
17.0262	66.0013	1264.4676	97.0029		
18.0352	6504.8960	21063.8234	1.0000		
22.9913	455978.5309	2084823.5888	40.0005	2032262.6821	26.0002
23.9843	542.0897	14301.2350	743.1685	15212.4049	714.1556
26.0148	3155.0358	52026.3577	13261.5262	53688.1127	10396.9186
27.0233	76671.3134	536084.9564	908.2517	535729.9026	582.1034
28.0187	5831.3651	24001.9545	92.0026	21611.9153	65.0013
28.0312	14540.3302	68572.1682	64.0013	66197.4825	48.0007
29.0028	65847.6662	364989.7575	1760.9460	336658.0049	1187.4302
29.0399	186753.4311	374481.1806	8.0000	367438.1770	4.0000
29.9981	24515.5023	495818.9592	7733.2217	476549.2521	6426.5876
30.0355	13315.9659	34928.6867	8.0000	29409.3778	8.0000
31.0189	88250.6581	412657.8088	1005.3084	374779.0682	813.2018
37.0060	472.0680	4720.7946	1001.3059	5127.0136	743.1685
38.0143	1106.3735	20372.1319	889.2413	20081.5668	710.1539
38.9655	28284.7500	65280.4146	1.0000	54068.4155	1.0000
39.0227	52279.2818	320261.4895	606.1121	328864.5364	398.0483
39.9605	794.1925	42016.1687	0.0000	38310.4324	0.0000
40.0304	13284.7132	56705.0582	826.2083	54005.3701	537.0880
41.0394	258207.3606	866719.0906	890.2418	839310.0869	508.0788
42.0103	20659.7105	77005.6303	21105.3545	71163.3428	15147.8091

Mass Interval Lists	posnew2 (+)	6	22.9913	2793823	7	23.9843	2002	8	26.0148	48788	9	27.0233	504621	10	28.0187	66699	11	28.0312	74139	12	29.0028	300321	
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Find:



Compilations

Spectra

CH\_30Be+ Mass (u) 40.0302 ?  Explained (%) 100.0 Corr. Area (cts) 60,498 Error (cts) 248 Resolution 5,302

Dev. (ppm) 5.1 ? Peak Difference... Poisson Corr. (%) 1.9 Error (%) 0.0 Width (ns) 2.06

Peak Statistics

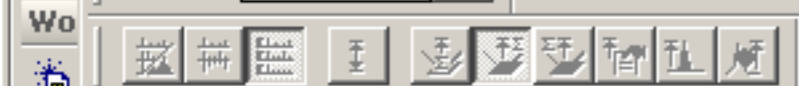
The 'Corrected Areas' button should be selected.

Ion	M	5100_01_	5100_06_	25100_01_	25500_01_	51000_01_
15.0000		3903.1592	143.0062	149607.3044	142110.7742	143044.6
15.9999		7510.1865	539516.0194	7760.3496	7785.4685	4317.6
17.0000		1589.7710	238737.7805	1637.8183	1602.7837	1022.0
17.0262	66.0013	1264.4878	97.0029	1470.6598	79.0019	1491.6788
18.0352	6504.8960	21063.8234	1.0000	37557.1931	0.0000	43510.6716
22.9913	455978.5309	2084823.5888	40.0005	2032262.6821	26.0002	2120615.7764
23.9843	542.0897	14301.2350	743.1685	15212.4049	714.1556	15300.2188
26.0148	3155.0358	52026.3577	13261.5262	53688.1127	10396.9186	57338.7328
27.0233	76671.3134	536084.9564	908.2517	535729.9026	582.1034	593138.1868
28.0187	5831.3651	24001.9545	92.0026	21611.9153	65.0013	21192.4718
28.0312	14540.3302	68572.1682	64.0013	66197.4825	48.0007	76905.0137
29.0028	65847.6662	364989.7575	1760.9460	336658.0049	1187.4302	364122.8091
29.0399	186753.4311	374481.1806	8.0000	367438.1770	4.0000	414047.7362
29.9981	24515.5023	495818.9592	7733.2217	476549.2521	6426.5876	518144.5731
30.0355	13315.9659	34928.6867	8.0000	29409.3778	8.0000	29951.1030
31.0189	88250.6581	412657.8088	1005.3084	374779.0682	813.2018	413271.5480
37.0060	472.0680	4720.7946	1001.3059	5127.0136	743.1685	5350.7278
38.0143	1106.3735	20372.1319	889.2413	20081.5668	710.1539	21680.8196
38.9655	28284.7500	65280.4146	1.0000	54068.4155	1.0000	64290.0167
39.0227	52279.2818	320261.4895	606.1121	328864.5364	398.0483	352194.6225
39.9605	794.1925	42016.1687	0.0000	38310.4324	0.0000	40879.7812
40.0304	13284.7132	56705.0582	826.2083	54005.3701	537.0880	59937.0824
41.0394	258207.3606	866719.0906	890.2418	839310.0869	508.0788	949671.0793
42.0103	20659.7105	77005.6303	21105.3545	71163.3428	15147.8091	76636.7327
					73606.9521	73606.9521

Mass Interval Lists	posnew2 (+)	6	22.9913	2793823	7	23.9843	2002	8	26.0148	48788	9	27.0233	504621	10	28.0187	66699	11	28.0312	74139	12	29.0028	300321	
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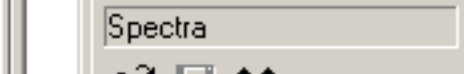
Find:



Compilations



Spectra



- 1100\_01\_1
- 1100\_02\_
- 1100\_06\_
- 5100\_01\_
- 5100\_06\_
- 25100\_01\_
- 25500\_01\_
- 51000\_01\_**

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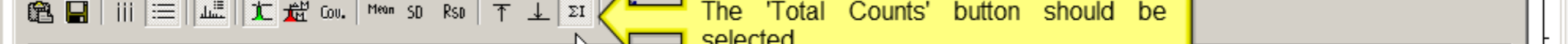
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Spectrum Properties

CH\_30Be+ Mass (u) 40.0302 ?  Explained (%) 100.0 Corr. Area (cts) 60,498 Error (cts) 248 Resolution 5,302  
 Check... Add Peak Dev. (ppm) 5.1 ? Peak Difference... Poisson Corr. (%) 1.9 Error (%) 0.0 Width (ns) 2.06



Peak Statistics



The 'Total Counts' button should be selected.

Ion	Mass	1100_01_1	1100_02_									
	15.0236	33461.3800	140278.4831									
	15.9940	33.0003	7493.1085									
	17.0019	4.0000	1634.8153									
	17.0262	66.0013	1264.4878									
	18.0352	6504.8960	21063.8234									
	22.9913	455978.5309	2084823.5888									
	23.9843	542.0897	14301.2350									
	26.0148	3155.0358	52026.3577									
	27.0233	76671.3134	536084.9564									
	28.0187	5831.3651	24001.9545									
	28.0312	14540.3302	68572.1682									
	29.0028	65847.6662	364989.7575									
	29.0399	186753.4311	374481.1806									
	29.9981	24515.5023	495818.9592									
	30.0355	13315.9659	34928.6867									
	31.0189	88250.6581	412657.8088									
	37.0060	472.0680	4720.7946									
	38.0143	1106.3735	20372.1319									
	38.9655	28284.7500	65280.4146									
	39.0227	52279.2818	320261.4895									
	39.9605	794.1925	42016.1687									
	40.0304	13284.7132	56705.0582									
	41.0394	258207.3606	866719.0906									
	42.0103	20659.7105	77005.6303									

<input checked="" type="checkbox"/>	6	22.9913	2793823									
<input checked="" type="checkbox"/>	7	23.9843	2002									
<input checked="" type="checkbox"/>	8	26.0148	48788									
<input checked="" type="checkbox"/>	9	27.0233	504621									
<input checked="" type="checkbox"/>	10	28.0187	66699									
<input checked="" type="checkbox"/>	11	28.0312	74139									
<input checked="" type="checkbox"/>	12	29.0028	300321									

Find:

Compilations

**Spectra**

- 1100\_01\_1
- 1100\_02\_
- 1100\_06\_
- 5100\_01\_
- 5100\_06\_
- 25100\_01\_
- 25500\_01\_
- 51000\_01**

Mass Interval Lists

- posnew2 (+)

Spectrum Properties

CH\_30Be+ Mass (u) 40.0302 ?  Explained (%) 100.0 Corr. Area (cts) 60,498 Error (cts) 248 Resolution 5,302

Dev. (ppm) 5.1 Peak Difference... Poisson Corr. (%) 1.9 Error (%) 0.0 Width (ns) 2.06

Peak Statistics

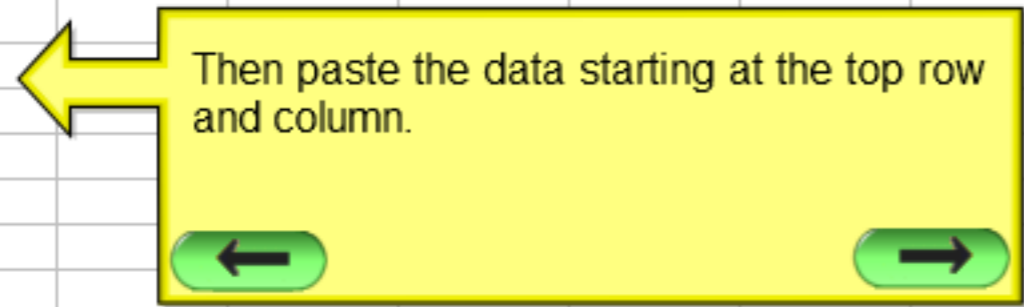
Once you have verified that the correct information is selected, press the 'Copy' button.

	1100_06_	5100_01_	5100_06_	25100_01_	25500_01_	51000_01_
195.0116	138903.1592	143.0062	149607.3044	142110.7742	143044.6	
648218.3548	7510.1865	539516.0194	7760.3496	7785.4685	4317.6	
286086.8354	1589.7710	238737.7805	1637.8183	1602.7837	1022.0	
97.0029	1470.6598	79.0019	1491.6788	1469.6590	3670.0	
18.0352	6504.8960	21063.8234	43510.6716	27598.1397	42710.0	
22.9913	455978.5309	2084823.5888	26.0002	2120615.7764	2934920.8630	
23.9843	542.0897	14301.2350	743.1685	15212.4049	714.1556	
26.0148	3155.0358	52026.3577	13261.5262	53688.1127	10396.9186	
27.0233	76671.3134	536084.9564	908.2517	535729.9026	582.1034	
28.0187	5831.3651	24001.9545	92.0026	21611.9153	65.0013	
28.0312	14540.3302	68572.1682	64.0013	66197.4825	48.0007	
29.0028	65847.6662	364989.7575	1760.9460	336658.0049	1187.4302	
29.0399	186753.4311	374481.1806	8.0000	367438.1770	4.0000	
29.9981	24515.5023	495818.9592	7733.2217	476549.2521	6426.5876	
30.0355	13315.9659	34928.6867	8.0000	29409.3778	8.0000	
31.0189	88250.6581	412657.8088	1005.3084	374779.0682	813.2018	
37.0060	472.0680	4720.7946	1001.3059	5127.0136	743.1685	
38.0143	1106.3735	20372.1319	889.2413	20081.5668	710.1539	
38.9655	28284.7500	65280.4146	1.0000	54068.4155	1.0000	
39.0227	52279.2818	320261.4895	606.1121	328864.5364	398.0483	
39.9605	794.1925	42016.1687	0.0000	38310.4324	0.0000	
40.0304	13284.7132	56705.0582	826.2083	54005.3701	537.0880	
41.0394	258207.3606	866719.0906	890.2418	839310.0869	508.0788	
42.0103	20659.7105	77005.6303	21105.3545	71163.3428	15147.8091	

	1100_06_	5100_01_	5100_06_	25100_01_	25500_01_	51000_01_
<input checked="" type="checkbox"/> 6	22.9913	2793823				
<input checked="" type="checkbox"/> 7	23.9843	2002				
<input checked="" type="checkbox"/> 8	26.0148	48788				
<input checked="" type="checkbox"/> 9	27.0233	504621				
<input checked="" type="checkbox"/> 10	28.0187	66699				
<input checked="" type="checkbox"/> 11	28.0312	74139				
<input checked="" type="checkbox"/> 12	29.0028	300321				

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
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Then paste the data starting at the top row and column.



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Date	: 10.11.2010															
2	Time	: 15:38:11															
3	File(s)	: 1100_01_1															
4		1100_02_															
5		1100_06_															
6		5100_01_															
7		5100_06_															
8		25100_01_															
9		25500_01_															
10		51000_01_															
11	lon	+	Mass														
12			1100_01_							25500_01_	51000_01_						
13		15.0236	33461.3							8	142110.8	143044.6					
14		15.994	33.000							5	7785.469	4317.684					
15		17.0019								8	1602.784	1022.319					
16		17.0262	66.000							9	1469.659	3670.108					
17		18.0352	6504.896	21063.82	1	37557.19	0	43510.67	27598.14		42710.9						
18		22.9913	455978.5	2084824	40.0005	2032263	26.0002	2120616	2934921		2793823						
19		23.9843	542.0897	14301.24	743.1685	15212.4	714.1556	15300.22	4710.766		2002.223						
20		26.0148	3155.036	52026.36	13261.53	53688.11	10396.92	57338.73	52428.99		48788.25						
21		27.0233	76671.31	536085	908.2517	535729.9	582.1034	593138.2	520893.6		504620.7						
22		28.0187	5831.365	24001.95	92.0026	21611.92	65.0013	21192.47	25907.76		66699.43						
23		28.0312	14540.33	68572.17	64.0013	66197.48	48.0007	76905.01	69490.04		74139.43						
24		29.0028	65847.67	364989.8	1760.946	336658	1187.43	364122.8	349239.1		300321.2						
25		29.0399	186753.4	374481.2	8	367438.2	4	414047.7	357022.1		346403.8						
26		29.9981	24515.5	495819	7733.222	476549.3	6426.588	518144.6	490149.9		405782.2						
27		30.0355	13315.97	34928.69	8	29409.38	8	29951.1	36942.37		96829.79						
28		31.0189	88250.66	412657.8	1005.308	374779.1	813.2018	413271.5	389597.1		339247.7						
29		37.006	472.068	4720.795	1001.306	5127.014	743.1685	5350.728	4942.447		4401.908						
30		38.0143	1106.374	20372.13	889.2413	20081.57	710.1539	21680.82	20082.58		20827.83						
31		38.9655	28284.75	65280.41	1	54068.42	1	64290.02	99202.57		84705.38						
32		39.0227	52279.28	320261.5	606.1121	328864.5	398.0483	352194.6	298491.7		286046.3						
33		39.9605	794.1925	42016.17	0	38310.43	0	40879.78	18564.78		9275.205						
34		40.0304	13284.71	56705.06	826.2083	54005.37	537.088	59937.08	54675.22		56746.47						
35		41.0394	258207.4	866719.1	890.2418	839310.1	508.0788	949671.1	796298.2		700251.8						
36		42.0103	20659.71	77005.63	21105.35	71163.34	15147.81	76636.73	73606.95		70709.1						
37		42.0449	26393.45	102303.5	1908.111	97391.09	1164.414	110455	95410.94		108875.7						
38		43.0195	123128.9	367378.1	7916.093	315930.2	5389.856	352989.5	341170.2		334071.2						
39		43.0552	158256.9	378839.3	975.2902	382461.1	484.0715	448399.6	354147.3		340292.3						
40		44.0267	42443.03	111373.1	688.1445	96147.78	526.0845	109688.1	104588.3		111289.6						
41		44.0514	7462.971	36156.03	96.0028	35960.77	61.0011	37292.21	43857.8		108948.4						
42		45.0351	110671.1	224522.8	5846.419	187122.2	3801.407	210962.2	199151.9		196157.6						
43		45.993	142414	1008338	324297.1	911658.3	244863.2	1043108	983091		813230.7						
44		47.0136	13196	58485.56	1065.346	48603.85	721.1587	54853.07	51021.24		50843.81						
45		48.0078	958.2802	12777.7	1643.824	11872.92	1251.478	13691.04	12119.72		13252.45						

Next move the 'lon' and 'Mass' titles one row down.

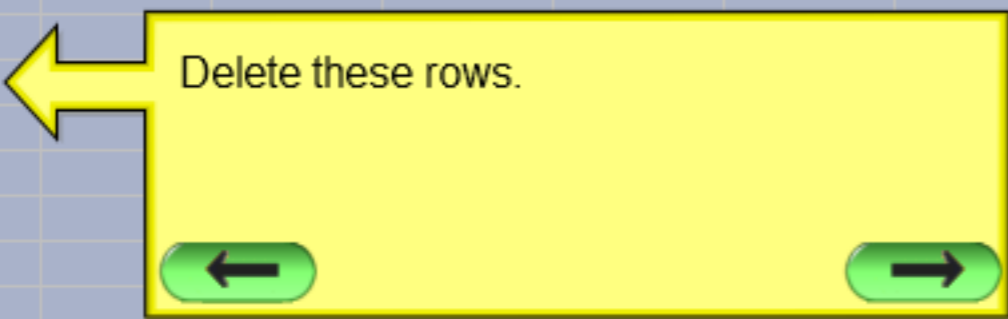
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	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
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2	Time	: 15:38:11															
3	File(s)	: 1100_01_1															
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6		5100_01_															
7		5100_06_															
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9		25500_01_															
10		51000_01_															
11																	
12	lon						5100_06_	25100_01_	25500_01_	51000_01_							
13							143.0062	149607.3	142110.8	143044.6							
14							539516	7760.35	7785.469	4317.684							
15							238737.8	1637.818	1602.784	1022.319							
16							79.0019	1491.679	1469.659	3670.108							
17		18.0352	6504.896	21063.82	1	37557.19	0	43510.67	27598.14	42710.9							
18		22.9913	455978.5	2084824	40.0005	2032263	26.0002	2120616	2934921	2793823							
19		23.9843	542.0897	14301.24	743.1685	15212.4	714.1556	15300.22	4710.766	2002.223							
20		26.0148	3155.036	52026.36	13261.53	53688.11	10396.92	57338.73	52428.99	48788.25							
21		27.0233	76671.31	536085	908.2517	535729.9	582.1034	593138.2	520893.6	504620.7							
22		28.0187	5831.365	24001.95	92.0026	21611.92	65.0013	21192.47	25907.76	66699.43							
23		28.0312	14540.33	68572.17	64.0013	66197.48	48.0007	76905.01	69490.04	74139.43							
24		29.0028	65847.67	364989.8	1760.946	336658	1187.43	364122.8	349239.1	300321.2							
25		29.0399	186753.4	374481.2	8	367438.2	4	414047.7	357022.1	346403.8							
26		29.9981	24515.5	495819	7733.222	476549.3	6426.588	518144.6	490149.9	405782.2							
27		30.0355	13315.97	34928.69	8	29409.38	8	29951.1	36942.37	96829.79							
28		31.0189	88250.66	412657.8	1005.308	374779.1	813.2018	413271.5	389597.1	339247.7							
29		37.006	472.068	4720.795	1001.306	5127.014	743.1685	5350.728	4942.447	4401.908							
30		38.0143	1106.374	20372.13	889.2413	20081.57	710.1539	21680.82	20082.58	20827.83							
31		38.9655	28284.75	65280.41	1	54068.42	1	64290.02	99202.57	84705.38							
32		39.0227	52279.28	320261.5	606.1121	328864.5	398.0483	352194.6	298491.7	286046.3							
33		39.9605	794.1925	42016.17	0	38310.43	0	40879.78	18564.78	9275.205							
34		40.0304	13284.71	56705.06	826.2083	54005.37	537.088	59937.08	54675.22	56746.47							
35		41.0394	258207.4	866719.1	890.2418	839310.1	508.0788	949671.1	796298.2	700251.8							
36		42.0103	20659.71	77005.63	21105.35	71163.34	15147.81	76636.73	73606.95	70709.1							
37		42.0449	26393.45	102303.5	1908.111	97391.09	1164.414	110455	95410.94	108875.7							
38		43.0195	123128.9	367378.1	7916.093	315930.2	5389.856	352989.5	341170.2	334071.2							
39		43.0552	158256.9	378839.3	975.2902	382461.1	484.0715	448399.6	354147.3	340292.3							
40		44.0267	42443.03	111373.1	688.1445	96147.78	526.0845	109688.1	104588.3	111289.6							
41		44.0514	7462.971	36156.03	96.0028	35960.77	61.0011	37292.21	43857.8	108948.4							
42		45.0351	110671.1	224522.8	5846.419	187122.2	3801.407	210962.2	199151.9	196157.6							
43		45.993	142414	1008338	324297.1	911658.3	244863.2	1043108	983091	813230.7							
44		47.0136	13196	58485.56	1065.346	48603.85	721.1587	54853.07	51021.24	50843.81							
45		48.0078	958.2802	12777.7	1643.824	11872.92	1251.478	13691.04	12119.72	13252.45							

Select all the rows above the titles you just moved.

A11

1	Date	: 10.11.2010
2	Time	: 15:38:11
3	File(s)	: 1100_01_1
4		1100_02_
5		1100_06_
6		5100_01_
7		5100_06_
8		25100_01_
9		25500_01_
10		51000_01_
11		



	Spectra:	Corrected Peak Intensity:								
12	Ion	Mass	1100_01_1	1100_02_	1100_06_	5100_01_	5100_06_	25100_01_	25500_01_	51000_01_
13		15.0236	33461.38	140278.5	195.0116	138903.2	143.0062	149607.3	142110.8	143044.6
14		15.994	33.0003	7493.109	648218.4	7510.187	539516	7760.35	7785.469	4317.684
15		17.0019	4	1634.815	286086.8	1589.771	238737.8	1637.818	1602.784	1022.319
16		17.0262	66.0013	1264.488	97.0029	1470.66	79.0019	1491.679	1469.659	3670.108
17		18.0352	6504.896	21063.82	1	37557.19	0	43510.67	27598.14	42710.9
18		22.9913	455978.5	2084824	40.0005	2032263	26.0002	2120616	2934921	2793823
19		23.9843	542.0897	14301.24	743.1685	15212.4	714.1556	15300.22	4710.766	2002.223
20		26.0148	3155.036	52026.36	13261.53	53688.11	10396.92	57338.73	52428.99	48788.25
21		27.0233	76671.31	536085	908.2517	535729.9	582.1034	593138.2	520893.6	504620.7
22		28.0187	5831.365	24001.95	92.0026	21611.92	65.0013	21192.47	25907.76	66699.43
23		28.0312	14540.33	68572.17	64.0013	66197.48	48.0007	76905.01	69490.04	74139.43
24		29.0028	65847.67	364989.8	1760.946	336658	1187.43	364122.8	349239.1	300321.2
25		29.0399	186753.4	374481.2	8	367438.2	4	414047.7	357022.1	346403.8
26		29.9981	24515.5	495819	7733.222	476549.3	6426.588	518144.6	490149.9	405782.2
27		30.0355	13315.97	34928.69	8	29409.38	8	29951.1	36942.37	96829.79
28		31.0189	88250.66	412657.8	1005.308	374779.1	813.2018	413271.5	389597.1	339247.7
29		37.006	472.068	4720.795	1001.306	5127.014	743.1685	5350.728	4942.447	4401.908
30		38.0143	1106.374	20372.13	889.2413	20081.57	710.1539	21680.82	20082.58	20827.83
31		38.9655	28284.75	65280.41	1	54068.42	1	64290.02	99202.57	84705.38
32		39.0227	52279.28	320261.5	606.1121	328864.5	398.0483	352194.6	298491.7	286046.3
33		39.9605	794.1925	42016.17	0	38310.43	0	40879.78	18564.78	9275.205
34		40.0304	13284.71	56705.06	826.2083	54005.37	537.088	59937.08	54675.22	56746.47
35		41.0394	258207.4	866719.1	890.2418	839310.1	508.0788	949671.1	796298.2	700251.8
36		42.0103	20659.71	77005.63	21105.35	71163.34	15147.81	76636.73	73606.95	70709.1
37		42.0449	26393.45	102303.5	1908.111	97391.09	1164.414	110455	95410.94	108875.7
38		43.0195	123128.9	367378.1	7916.093	315930.2	5389.856	352989.5	341170.2	334071.2
39		43.0552	158256.9	378839.3	975.2902	382461.1	484.0715	448399.6	354147.3	340292.3
40		44.0267	42443.03	111373.1	688.1445	96147.78	526.0845	109688.1	104588.3	111289.6
41		44.0514	7462.971	36156.03	96.0028	35960.77	61.0011	37292.21	43857.8	108948.4
42		45.0351	110671.1	224522.8	5846.419	187122.2	3801.407	210962.2	199151.9	196157.6
43		45.993	142414	1008338	324297.1	911658.3	244863.2	1043108	983091	813230.7
44		47.0136	13196	58485.56	1065.346	48603.85	721.1587	54853.07	51021.24	50843.81
45		48.0078	958.2802	12777.7	1643.824	11872.92	1251.478	13691.04	12119.72	13252.45



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Ion	Mass	1100_01	1100_02	1100_06	5100_01	5100_06	25100_01	25500_01	51000_01							
2		15.0236	33461.38	140278.5	195.0116	138903.2	143.0062	149607.3	142110.8	143044.6							
3		15.994						7760.35	7785.469	4317.684							
4								1637.818	1602.784	1022.319							
5		17.0262						1491.679	1469.659	3670.108							
6		18.0352						43510.67	27598.14	42710.9							
7		22.9913						2120616	2934921	2793823							
8		23.9843						15300.22	4710.766	2002.223							
9		26.0148						57338.73	52428.99	48788.25							
10		27.0233						593138.2	520893.6	504620.7							
11		28.0187						21192.47	25907.76	66699.43							
12		28.0312						76905.01	69490.04	74139.43							
13		29.0028						364122.8	349239.1	300321.2							
14		29.0399						414047.7	357022.1	346403.8							
15		29.9981						518144.6	490149.9	405782.2							
16		30.0355						29951.1	36942.37	96829.79							
17		31.0189						413271.5	389597.1	339247.7							
18		37.006						5350.728	4942.447	4401.908							
19		38.0143						21680.82	20082.58	20827.83							
20		38.9655						64290.02	99202.57	84705.38							
21		39.0227						352194.6	298491.7	286046.3							
22		39.9605	794.1925	42016.17	0	38310.43	0	40879.78	18564.78	9275.205							
23		40.0304	13284.71	56705.06	826.2083	54005.37	537.088	59937.08	54675.22	56746.47							
24		41.0394	258207.4	866719.1	890.2418	839310.1	508.0788	949671.1	796298.2	700251.8							
25		42.0103	20659.71	77005.63	21105.35	71163.34	15147.81	76636.73	73606.95	70709.1							
26		42.0449	26393.45	102303.5	1908.111	97391.09	1164.414	110455	95410.94	108875.7							
27		43.0195	123128.9	367378.1	7916.093	315930.2	5389.856	352989.5	341170.2	334071.2							
28		43.0552	158256.9	378839.3	975.2902	382461.1	484.0715	448399.6	354147.3	340292.3							
29		44.0267	42443.03	111373.1	688.1445	96147.78	526.0845	109688.1	104588.3	111289.6							
30		44.0514	7462.971	36156.03	96.0028	35960.77	61.0011	37292.21	43857.8	108948.4							
31		45.0351	110671.1	224522.8	5846.419	187122.2	3801.407	210962.2	199151.9	196157.6							
32		45.993	142414	1008338	324297.1	911658.3	244863.2	1043108	983091	813230.7							
33		47.0136	13196	58485.56	1065.346	48603.85	721.1587	54853.07	51021.24	50843.81							
34		48.0078	958.2802	12777.7	1643.824	11872.92	1251.478	13691.04	12119.72	13252.45							
35		49.0312	1070.35	2607.073	337.0347	2064.3	248.0188	2521.94	2289.599	2116.366							
36		50.0135	961.2819	8418.592	529.0854	8698.048	398.0483	8825.729	8843.826	11357.27							
37		51.0226	4841.145	34527.27	460.0646	33095.01	310.0293	35062.51	32608.35	37066.14							
38		51.9378	313.0299	14739.1	7	2848.475	0	15467.78	1556.739	10952.53							
39		52.0303	2967.686	21598.74	253.0195	19658.47	215.0141	21572.4	19343.74	22590.02							
40		53.0019	14963.12	48000.32	1998.218	41543.26	1376.578	46413.24	54782.76	55099.19							
41		53.0394	35994.51	135494.3	297.0269	119280.5	190.011	134813.4	116833.4	119638.7							
42		54.0107	5764.128	31252.18	336.0345	26731.9	246.0185	29849.26	28327.48	29571.27							
43		54.0461	7119.446	52651	150.0069	47665.69	102.0032	56208.23	46045	50962.44							
44		55.019	58489.71	236076.8	4876.249	199392.4	3272.266	223120.7	213382.2	266717							
45		55.0555	82962.45	290683.8	680.1412	273360.4	416.0528	330637.8	259937.4	250321.8							

All rows in the 'Ion' column must have an entry. If you entered identities for the peaks in your table within the Ionof software, those entries will already be there.

If there are any blank rows, you must enter something in order for my import function to work.

You can either enter an identity that you have determined or just enter a place holder.

For the tutorial we will just enter 'unknown' for each row.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Ion	Mass	1100_01_	1100_02_	1100_06_	5100_01_	5100_06_	25100_01_	25500_01_	51000_01_							
2	unknown	15.0236	33461.38	140278.5	195.0116	138903.2	143.0062	149607.3	142110.8	143044.6							
3		15.994	33461.38	140278.5	195.0116	138903.2	143.0062	149607.3	142110.8	143044.6							
4		15.994	33461.38	140278.5	195.0116	138903.2	143.0062	149607.3	142110.8	143044.6							
5		15.994	33461.38	140278.5	195.0116	138903.2	143.0062	149607.3	142110.8	143044.6							
6		18.0352	33461.38	140278.5	195.0116	138903.2	143.0062	149607.3	142110.8	143044.6							
7		22.9913	33461.38	140278.5	195.0116	138903.2	143.0062	149607.3	142110.8	143044.6							
8		23.9843	33461.38	140278.5	195.0116	138903.2	143.0062	149607.3	142110.8	143044.6							
9		26.0148	33461.38	140278.5	195.0116	138903.2	143.0062	149607.3	142110.8	143044.6							
10		27.0233	33461.38	140278.5	195.0116	138903.2	143.0062	149607.3	142110.8	143044.6							
11		28.0187	33461.38	140278.5	195.0116	138903.2	143.0062	149607.3	142110.8	143044.6							
12		28.0312	33461.38	140278.5	195.0116	138903.2	143.0062	149607.3	142110.8	143044.6							
13		29.0028	65847.67	364989.8	1760.946	336658	1187.43	364122.8	349239.1	300321.2							
14		29.0399	186753.4	374481.2	8	367438.2	4	414047.7	357022.1	346403.8							
15		29.9981	24515.5	495819	7733.222	476549.3	6426.588	518144.6	490149.9	405782.2							
16		30.0355	13315.97	34928.69	8	29409.38	8	29951.1	36942.37	96829.79							
17		31.0189	88250.66	412657.8	1005.308	374779.1	813.2018	413271.5	389597.1	339247.7							
18		37.006	472.068	4720.795	1001.306	5127.014	743.1685	5350.728	4942.447	4401.908							
19		38.0143	1106.374	20372.13	889.2413	20081.57	710.1539	21680.82	20082.58	20827.83							
20		38.9655	28284.75	65280.41	1	54068.42	1	64290.02	99202.57	84705.38							
21		39.0227	52279.28	320261.5	606.1121	328864.5	398.0483	352194.6	298491.7	286046.3							
22		39.9605	794.1925	42016.17	0	38310.43	0	40879.78	18564.78	9275.205							
23		40.0304	13284.71	56705.06	826.2083	54005.37	537.088	59937.08	54675.22	56746.47							
24		41.0394	258207.4	866719.1	890.2418	839310.1	508.0788	949671.1	796298.2	700251.8							
25		42.0103	20659.71	77005.63	21105.35	71163.34	15147.81	76636.73	73606.95	70709.1							
26		42.0449	26393.45	102303.5	1908.111	97391.09	1164.414	110455	95410.94	108875.7							
27		43.0195	123128.9	367378.1	7916.093	315930.2	5389.856	352989.5	341170.2	334071.2							
28		43.0552	158256.9	378839.3	975.2902	382461.1	484.0715	448399.6	354147.3	340292.3							
29		44.0267	42443.03	111373.1	688.1445	96147.78	526.0845	109688.1	104588.3	111289.6							
30		44.0514	7462.971	36156.03	96.0028	35960.77	61.0011	37292.21	43857.8	108948.4							
31		45.0351	110671.1	224522.8	5846.419	187122.2	3801.407	210962.2	199151.9	196157.6							
32		45.993	142414	1008338	324297.1	911658.3	244863.2	1043108	983091	813230.7							
33		47.0136	13196	58485.56	1065.346	48603.85	721.1587	54853.07	51021.24	50843.81							
34		48.0078	958.2802	12777.7	1643.824	11872.92	1251.478	13691.04	12119.72	13252.45							
35		49.0312	1070.35	2607.073	337.0347	2064.3	248.0188	2521.94	2289.599	2116.366							
36		50.0135	961.2819	8418.592	529.0854	8698.048	398.0483	8825.729	8843.826	11357.27							
37		51.0226	4841.145	34527.27	460.0646	33095.01	310.0293	35062.51	32608.35	37066.14							
38		51.9378	313.0299	14739.1	7	2848.475	0	15467.78	1556.739	10952.53							
39		52.0303	2967.686	21598.74	253.0195	19658.47	215.0141	21572.4	19343.74	22590.02							
40		53.0019	14963.12	48000.32	1998.218	41543.26	1376.578	46413.24	54782.76	55099.19							
41		53.0394	35994.51	135494.3	297.0269	119280.5	190.011	134813.4	116833.4	119638.7							
42		54.0107	5764.128	31252.18	336.0345	26731.9	246.0185	29849.26	28327.48	29571.27							
43		54.0461	7119.446	52651	150.0069	47665.69	102.0032	56208.23	46045	50962.44							
44		55.019	58489.71	236076.8	4876.249	199392.4	3272.266	223120.7	213382.2	266717							
45		55.0555	82962.45	290683.8	680.1412	273360.4	416.0528	330637.8	259937.4	250321.8							

I will copy and paste 'unknown' into all the rows.

NOTE: Do not use spaces in the labels in the ion column. If there are any spaces the file will not import properly.

Now save the file as a tab delimited text file.

	A	B	H	I	J	K	L	M	N	O	P	Q
1	lon	Mas	06	25100_01	25500_01	51000_01						
2	unknown	15	0062	149607.3	142110.8	143044.6						
3	unknown	15.994	33.0003	7493.109	648218.4	7510.187	539516	7760.35	7785.469	4317.684		
4	unknown	17.0019	4	1634.815	286086.8	1589.771	238737.8	1637.818	1602.784	1022.319		
5	unknown	17.0262	66.0013	1264.488	97.0029	1470.66	79.0019	1491.679	1469.659	3670.108		
6	unknown	18.0352	6504.896	21063.82	1	37557.19	0	43510.67	27598.14	42710.9		
7	unknown	22.9913	455978.5	2084824	40.0005	2032263	26.0002	2120616	2934921	2793823		
8	unknown	23.9843	542.0897	14301.24	743.1685	15212.4	714.1556	15300.22	4710.766	2002.223		
9	unknown	26.0148	3155.036	52026.36	13261.53	53688.11	10396.92	57338.73	52428.99	48788.25		
10	unknown	27.0233	76671.31	536085	908.2517	535729.9	582.1034	593138.2	520893.6	504620.7		
11	unknown	28.0187	5831.365	24001.95	92.0026	21611.92	65.0013	21192.47	25907.76	66699.43		
12	unknown	28.0312	14540.33	68572.17	64.0013	66197.48	48.0007	76905.01	69490.04	74139.43		
13	unknown	29.0028	65847.67	364989.8	1760.946	336658	1187.43	364122.8	349239.1	300321.2		
14	unknown	29.0399	186753.4	374481.2	8	367438.2	4	414047.7	357022.1	346403.8		
15	unknown	29.9981	24515.5	495819	7733.222	476549.3	6426.588	518144.6	490149.9	405782.2		
16	unknown	30.0355	13315.97	34928.69	8	29409.38	8	29951.1	36942.37	96829.79		
17	unknown	31.0189	88250.66	412657.8	1005.308	374779.1	813.2018	413271.5	389597.1	339247.7		
18	unknown	37.006	472.068	4720.795	1001.306	5127.014	743.1685	5350.728	4942.447	4401.908		
19	unknown	38.0143	1106.374	20372.13	889.2413	20081.57	710.1539	21680.82	20082.58	20827.83		
20	unknown	38.9655	28284.75	65280.41	1	54068.42	1	64290.02	99202.57	84705.38		
21	unknown	39.0227	52279.28	320261.5	606.1121	328864.5	398.0483	352194.6	298491.7	286046.3		
22	unknown	39.9605	794.1925	42016.17	0	38310.43	0	40879.78	18564.78	9275.205		
23	unknown	40.0304	13284.71	56705.06	826.2083	54005.37	537.088	59937.08	54675.22	56746.47		
24	unknown	41.0394	258207.4	866719.1	890.2418	839310.1	508.0788	949671.1	796298.2	700251.8		
25	unknown	42.0103	20659.71	77005.63	21105.35	71163.34	15147.81	76636.73	73606.95	70709.1		
26	unknown	42.0449	26393.45	102303.5	1908.111	97391.09	1164.414	110455	95410.94	108875.7		
27	unknown	43.0195	123128.9	367378.1	7916.093	315930.2	5389.856	352989.5	341170.2	334071.2		
28	unknown	43.0552	158256.9	378839.3	975.2902	382461.1	484.0715	448399.6	354147.3	340292.3		
29	unknown	44.0267	42443.03	111373.1	688.1445	96147.78	526.0845	109688.1	104588.3	111289.6		
30	unknown	44.0514	7462.971	36156.03	96.0028	35960.77	61.0011	37292.21	43857.8	108948.4		
31	unknown	45.0351	110671.1	224522.8	5846.419	187122.2	3801.407	210962.2	199151.9	196157.6		
32	unknown	45.993	142414	1008338	324297.1	911658.3	244863.2	1043108	983091	813230.7		
33	unknown	47.0136	13196	58485.56	1065.346	48603.85	721.1587	54853.07	51021.24	50843.81		
34	unknown	48.0078	958.2802	12777.7	1643.824	11872.92	1251.478	13691.04	12119.72	13252.45		
35	unknown	49.0312	1070.35	2607.073	337.0347	2064.3	248.0188	2521.94	2289.599	2116.366		
36	unknown	50.0135	961.2819	8418.592	529.0854	8698.048	398.0483	8825.729	8843.826	11357.27		
37	unknown	51.0226	4841.145	34527.27	460.0646	33095.01	310.0293	35062.51	32608.35	37066.14		
38	unknown	51.9378	313.0299	14739.1	7	2848.475	0	15467.78	1556.739	10952.53		
39	unknown	52.0303	2967.686	21598.74	253.0195	19658.47	215.0141	21572.4	19343.74	22590.02		
40	unknown	53.0019	14963.12	48000.32	1998.218	41543.26	1376.578	46413.24	54782.76	55099.19		
41	unknown	53.0394	35994.51	135494.3	297.0269	119280.5	190.011	134813.4	116833.4	119638.7		
42	unknown	54.0107	5764.128	31252.18	336.0345	26731.9	246.0185	29849.26	28327.48	29571.27		
43	unknown	54.0461	7119.446	52651	150.0069	47665.69	102.0032	56208.23	46045	50962.44		
44	unknown	55.019	58489.71	236076.8	4876.249	199392.4	3272.266	223120.7	213382.2	266717		
45	unknown	55.0555	82962.45	290683.8	680.1412	273360.4	416.0528	330637.8	259937.4	250321.8		

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Ion	Mass	1100_01_1	1100_02_	1100_06_	5100_01_	5100_06_	25100_01_	25500_01_	51000_01_							
2	unknown	15.0236	33461.38	140278.5	195.0116	138903.2	143.0062	149607.3	142110.8	143044.6							
3	unknown	15.994	33.0003	7493.109	648218.4	7510.187	539516	7760.35	7785.469	4317.684							
4	unknown	17.0019	4	1634.815	286086.8	1589.771	238737.8	1637.818	1602.784	1022.319							
5	unknown	17.0262	66.0013	1264.488	97.0029	1470.66	79.0019	1491.679	1469.659	3670.108							
6	unknown	18.0352	6504.896	21063.82	1	37557.19	0	43510.67	27598.14	42710.9							
7	unknown	22.9913	455978.5	2084824	40.0005	2032263	26.0002	2120616	2934921	2793823							
8	unknown	23.9843	542.0897	14301.24	743.1685	15212.4	714.1556	15300.22	4710.766	2002.223							
9	unknown	26.0148	3155.036	52026.36	13261.53	53688.11	10396.92	57338.73	52428.99	48788.25							
10	unknown	27.0233	76671.31	536085	908.2517	535729.9	582.1034	593138.2	520893.6	504620.7							
11	unknown	28.0187	5831.365	24001.95	92.0026	21611.92	65.0013	21192.47	25907.76	66699.43							
12	unknown	28.0312	14540.33	68572.17	64.0013	66197.48	48.0007	76905.01	69490.04	74139.43							
13	unknown	29.0028	65847.67	364989.8	1760.946	336658											
14	unknown	29.0399	186753.4	374481.2	8	367438.2											
15	unknown	29.9981	24515.5	495819	7733.222	476549.3											
16	unknown	30.0355	13315.97	34928.69	8	29409.38											
17	unknown	31.0189	88250.66	412657.8	1005.308	374779.1											
18	unknown	37.006	472.068	4720.795	1001.306	5127.014											
19	unknown	38.0143	1106.374	20372.13	889.2413	20081.57											
20	unknown	38.9655	28284.75	65280.41	1	54068.42											
21	unknown	39.0227	52279.28	320261.5	606.1121	328864.5											
22	unknown	39.9605	794.1925	42016.17	0	38310.43											
23	unknown	40.0304	13284.71	56705.06	826.2083	54005.37											
24	unknown	41.0394	258207.4	866719.1	890.2418	839310.1											
25	unknown	42.0103	20659.71	77005.63	21105.35	71163.34											
26	unknown	42.0449	26393.45	102303.5	1908.111	97391.09											
27	unknown	43.0195	123128.9	367378.1	7916.093	315930.2											
28	unknown	43.0552	158256.9	378839.3	975.2902	382461.1											
29	unknown	44.0267	42443.03	111373.1	688.1445	96147.78											
30	unknown	44.0514	7462.971	36156.03	96.0028	35960.77											
31	unknown	45.0351	110671.1	224522.8	5846.419	187122.2											
32	unknown	45.993	142414	1008338	324297.1	911658.3											
33	unknown	47.0136	13196	58485.56	1065.346	48603.85											
34	unknown	48.0078	958.2802	12777.7	1643.824	11872.92											
35	unknown	49.0312	1070.35	2607.073	337.0347	2064.3											
36	unknown	50.0135	961.2819	8418.592	529.0854	8698.048	398.0483	8825.729	8843.826	11357.27							
37	unknown	51.0226	4841.145	34527.27	460.0646	33095.01	310.0293	35062.51	32608.35	37066.14							
38	unknown	51.9378	313.0299	14739.1	7	2848.475	0	15467.78	1556.739	10952.53							
39	unknown	52.0303	2967.686	21598.74	253.0195	19658.47	215.0141	21572.4	19343.74	22590.02							
40	unknown	53.0019	14963.12	48000.32	1998.218	41543.26	1376.578	46413.24	54782.76	55099.19							
41	unknown	53.0394	35994.51	135494.3	297.0269	119280.5	190.011	134813.4	116833.4	119638.7							
42	unknown	54.0107	5764.128	31252.18	336.0345	26731.9	246.0185	29849.26	28327.48	29571.27							
43	unknown	54.0461	7119.446	52651	150.0069	47665.69	102.0032	56208.23	46045	50962.44							
44	unknown	55.019	58489.71	236076.8	4876.249	199392.4	3272.266	223120.7	213382.2	266717							
45	unknown	55.0555	82962.45	290683.8	680.1412	273360.4	416.0528	330637.8	259937.4	250321.8							

**Save As**

Save in: work

- allpeaksimpos.txt
- asbposdata.txt
- CH3NEV.TXT
- controldata.txt
- fortutorial.txt
- FRE-HYD-old.TXT
- iontof.txt
- it6files.txt
- loads.txt
- loads\_rescaled.txt
- negative.txt
- negnewdata.txt
- newch.txt
- NHS-BARE.TXT
- positive.txt
- redpos.txt
- scores.txt
- TEST2.TXT
- testv6.txt
- variance.txt

File name: testv6.txt

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

Buttons: Save, Cancel

Choose where you want to save the file.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	
1	Ion	Mass	1100_01_1	1100_02_	1100_06_	5100_01_	5100_06_	25100_01_	25500_01_	51000_01_								
2	unknown	15.0236	33461.38	140278.5	195.0116	138903.2	143.0062	149607.3	142110.8	143044.6								
3	unknown	15.994	33.0003	7493.109	648218.4	7510.187	539516	7760.35	7785.469	4317.684								
4	unknown	17.0019	4	1634.815	286086.8	1589.771	238737.8	1637.818	1602.784	1022.319								
5	unknown	17.0262	66.0013	1264.488	97.0029	1470.66	79.0019	1491.679	1469.659	3670.108								
6	unknown	18.0352	6504.896	21063.82	1	37557.19	0	43510.67	27598.14	42710.9								
7	unknown	22.9913	455978.5	2084824	40.0005	2032263	26.0002	2120616	2934921	2793823								
8	unknown	23.9843	542.0897	14301.24	743.1685	15212.4	714.1556	15300.22	4710.766	2002.223								
9	unknown	26.0148	3155.036	52026.36	13261.53	53688.11	10396.92	57338.73	52428.99	48788.25								
10	unknown	27.0233	76671.31	536085	908.2517	535729.9	582.1034	593138.2	520893.6	504620.7								
11	unknown	28.0187	5831.365	24001.95	92.0026	21611.92	65.0013	21192.47	25907.76	66699.43								
12	unknown	28.0312	14540.33	68572.17	64.0013	66197.48	48.0007	76905.01	69490.04	74139.43								
13	unknown	29.0028	65847.67	364989.8	1760.946	336658												
14	unknown	29.0399	186753.4	374481.2	8	367438.2												
15	unknown	29.9981	24515.5	495819	7733.222	476549.3												
16	unknown	30.0355	13315.97	34928.69	8	29409.38												
17	unknown	31.0189	88250.66	412657.8	1005.308	374779.1												
18	unknown	37.006	472.068	4720.795	1001.306	5127.014												
19	unknown	38.0143	1106.374	20372.13	889.2413	20081.57												
20	unknown	38.9655	28284.75	65280.41	1	54068.42												
21	unknown	39.0227	52279.28	320261.5	606.1121	328864.5												
22	unknown	39.9605	794.1925	42016.17	0	38310.43												
23	unknown	40.0304	13284.71	56705.06	826.2083	54005.37												
24	unknown	41.0394	258207.4	866719.1	890.2418	839310.1												
25	unknown	42.0103	20659.71	77005.63	21105.35	71163.34												
26	unknown	42.0449	26393.45	102303.5	1908.111	97391.09												
27	unknown	43.0195	123128.9	367378.1	7916.093	315930.2												
28	unknown	43.0552	158256.9	378839.3	975.2902	382461.1												
29	unknown	44.0267	42443.03	111373.1	688.1445	96147.78												
30	unknown	44.0514	7462.971	36156.03	96.0028	35960.77												
31	unknown	45.0351	110671.1	224522.8	5846.419	187122.2												
32	unknown	45.993	142414	1008338	324297.1	911658.3												
33	unknown	47.0199	12499	59495.58	4895.248	48992.95												
34	unknown	48.0					483	8825.729	8843.826	11357.27								
35	unknown	49.0					293	35062.51	32608.35	37066.14								
36	unknown	50.0					0	15467.78	1556.739	10952.53								
37	unknown	51.0					141	21572.4	19343.74	22590.02								
38	unknown	51.9					578	46413.24	54782.76	55099.19								
39	unknown	52.0																
40	unknown	53.0																
41	unknown	53.0394	35994.51	135494.3	297.0269	119280.5	190.011	134813.4	116833.4	119638.7								
42	unknown	54.0107	5764.128	31252.18	336.0345	26731.9	246.0185	29849.26	28327.48	29571.27								
43	unknown	54.0461	7119.446	52651	150.0069	47665.69	102.0032	56208.23	46045	50962.44								
44	unknown	55.019	58489.71	236076.8	4876.249	199392.4	3272.266	223120.7	213382.2	266717								
45	unknown	55.0555	82962.45	290683.8	680.1412	273360.4	416.0528	330637.8	259937.4	250321.8								

**Save As**

Save in: fortutorial

History

My Documents

Desktop

Favorites

File name: testv6.txt

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

Save Cancel

Make sure the file type is 'Text (Tab delimited) (\*.txt)'

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Ion	Mass	1100_01_1	1100_02_	1100_06_	5100_01_	5100_06_	25100_01_	25500_01_	51000_01_							
2	unknown	15.0236	33461.38	140278.5	195.0116	138903.2	143.0062	149607.3	142110.8	143044.6							
3	unknown	15.994	33.0003	7493.109	648218.4	7510.187	539516	7760.35	7785.469	4317.684							
4	unknown	17.0019	4	1634.815	286086.8	1589.771	238737.8	1637.818	1602.784	1022.319							
5	unknown	17.0262	66.0013	1264.488	97.0029	1470.66	79.0019	1491.679	1469.659	3670.108							
6	unknown	18.0352	6504.896	21063.82	1	37557.19	0	43510.67	27598.14	42710.9							
7	unknown	22.9913	455978.5	2084824	40.0005	2032263	26.0002	2120616	2934921	2793823							
8	unknown	23.9843	542.0897	14301.24	743.1685	15212.4	714.1556	15300.22	4710.766	2002.223							
9	unknown	26.0148	3155.036	52026.36	13261.53	53688.11	10396.92	57338.73	52428.99	48788.25							
10	unknown	27.0233	76671.31	536085	908.2517	535729.9	582.1034	593138.2	520893.6	504620.7							
11	unknown	28.0187	5831.365	24001.95	92.0026	21611.92	65.0013	21192.47	25907.76	66699.43							
12	unknown	28.0312	14540.33	68572.17	64.0013	66197.48	48.0007	76905.01	69490.04	74139.43							
13	unknown	29.0028	65847.67	364989.8	1760.946	336658											
14	unknown	29.0399	186753.4	374481.2	8	367438.2											
15	unknown	29.9981	24515.5	495819	7733.222	476549.3											
16	unknown	30.0355	13315.97	34928.69	8	29409.38											
17	unknown	31.0189	88250.66	412657.8	1005.308	374779.1											
18	unknown	37.006	472.068	4720.795	1001.306	5127.014											
19	unknown	38.0143	1106.374	20372.13	889.2413	20081.57											
20	unknown	38.9655	28284.75	65280.41	1	54068.42											
21	unknown	39.0227	52279.28	320261.5	606.1121	328864.5											
22	unknown	39.9605	794.1925	42016.17	0	38310.43											
23	unknown	40.0304	13284.71	56705.06	826.2083	54005.37											
24	unknown	41.0394	258207.4	866719.1	890.2418	839310.1											
25	unknown	42.0103	20659.71	77005.63	21105.35	71163.34											
26	unknown	42.0449	26393.45	102303.5	1908.111	97391.09											
27	unknown	43.0195	123128.9	367378.1	7916.093	315930.2											
28	unknown	43.0552	158256.9	378839.3	975.2902	382461.1											
29	unknown	44.0267	42443.03	111373.1	688.1445	96147.78											
30	unknown	44.0514	7462.971	36156.03	96.0028	35960.77											
31	unknown	45.0351	110671.1	224522.8	5846.419	187122.2											
32	unknown	45.993															
33	unknown	47.0136															
34	unknown	48.0078															
35	unknown	49.0312															
36	unknown	50.0135															
37	unknown	51.0226															
38	unknown	51.9378															
39	unknown	52.0303															
40	unknown	53.0019															
41	unknown	53.0394															
42	unknown	54.0107															
43	unknown	54.0461															
44	unknown	55.019															
45	unknown	55.0555															

**Save As**

Save in: fortutorial

History

My Documents

Desktop

Favorites

File name: testv6.txt

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

Save

Cancel

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

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Ion	Mass	1100_01_1	1100_02_	1100_06_	5100_01_	5100_06_	25100_01_	25500_01_	51000_01_							
2	unknown	15.0236	33461.38	140278.5	195.0116	138903.2	143.0062	149607.3	142110.8	143044.6							
3	unknown	15.994	33.0003	7493.109	648218.4	7510.187	539516	7760.35	7785.469	4317.684							
4	unknown	17.0019	4	1634.815	286086.8	1589.771	238737.8	1637.818	1602.784	1022.319							
5	unknown	17.0262	66.0013	1264.488	97.0029	1470.66	79.0019	1491.679	1469.659	3670.108							
6	unknown	18.0352	6504.896	21063.82	1	37557.19	0	43510.67	27598.14	42710.9							
7	unknown	22.9913	455978.5	2084824	40.0005	2032263	26.0002	2120616	2934921	2793823							
8	unknown	23.9843	542.0897	14301.24	743.1685	15212.4	714.1556	15300.22	4710.766	2002.223							
9	unknown	26.0148	3155.036	52026.36	13261.53	53688.11	10396.92	57338.73	52428.99	48788.25							
10	unknown	27.0233	76671.31	536085	908.2517	535729.9	582.1034	593138.2	520893.6	504620.7							
11	unknown	28.0187	5831.365	24001.95	92.0026	21611.92	65.0013	21192.47	25907.76	66699.43							
12	unknown	28.0312	14540.33	68572.17	64.0013	66197.48	48.0007	76905.01	69490.04	74139.43							
13	unknown	29.0028	65847.67	364989.8	1760.946	336658											
14	unknown	29.0399	186753.4	374481.2	8	367438.2											
15	unknown	29.9981	24515.5	495819	7733.222	476549.3											
16	unknown	30.0355	13315.97	34928.69	8	29409.38											
17	unknown	31.0189	88250.66	412657.8	1005.308	374779.1											
18	unknown	37.006	472.068	4720.795	1001.306	5127.014											
19	unknown	38.0143	1106.374	20372.13	889.2413	20081.57											
20	unknown	38.9655	28284.75	65280.41	1	54068.42											
21	unknown	39.0227	52279.28	320261.5	606.1121	328864.5											
22	unknown	39.9605	794.1925	42016.17	0	38310.43											
23	unknown	40.0304	13284.71	56705.06	826.2083	54005.37											
24	unknown	41.0394	258207.4	866719.1	890.2418	839310.1											
25	unknown	42.0103	20659.71	77005.63	21105.35	71163.34											
26	unknown	42.0449	26393.45	102303.5	1908.111	97391.09											
27	unknown	43.0195	123128.9	367378.1	7916.093	315930.2											
28	unknown	43.0552	158256.9	378839.3	975.2902	382461.1											
29	unknown	44.0267	42443.03	111373.1	688.1445	96147.78											
30	unknown	44.0514	7462.971	36156.03	96.0028	35960.77											
31	unknown	45.0351	110671.1	224522.8	5846.419	187122.2											
32	unknown	45.993	142414	1008338	324297.1	911658.3											
33	unknown	47.0136	13196	58485.56	1065.346	48603.85											
34	unknown	48.0078	958.2802	12777.7	1643.824	11872.92											
35	unknown	49.0312	1070.35	2607.073	337.0347	2064.3											
36	unknown	50.0135	961.2819	8418.592	529.0854	8698.048	398.0483	8825									
37	unknown	51.0226	4841.145	34527.27	460.0646	33095.01	310.0293	3506									
38	unknown	51.9378	313.0299	14739.1	7	2848.475	0	1546									
39	unknown	52.0303	2967.686	21598.74	253.0195	19658.47	215.0141	21572.4	19343.74	22590.02							
40	unknown	53.0019	14963.12	48000.32	1998.218	41543.26	1376.578	46413.24	54782.76	55099.19							
41	unknown	53.0394	35994.51	135494.3	297.0269	119280.5	190.011	134813.4	116833.4	119638.7							
42	unknown	54.0107	5764.128	31252.18	336.0345	26731.9	246.0185	29849.26	28327.48	29571.27							
43	unknown	54.0461	7119.446	52651	150.0069	47665.69	102.0032	56208.23	46045	50962.44							
44	unknown	55.019	58489.71	236076.8	4876.249	199392.4	3272.266	223120.7	213382.2	266717							
45	unknown	55.0555	82962.45	290683.8	680.1412	273360.4	416.0528	330637.8	259937.4	250321.8							

**Save As**

Save in: fortutorial

- History
- My Documents
- Desktop
- Favorites
- My Network Places

Press the 'Save' button to save the file.

Save Cancel

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Ion	Mass	1100_01_1	1100_02_	1100_06_	5100_01_	5100_06_	25100_01_	25500_01_	51000_01_							
2	unknown	15.0236	33461.38	140278.5	195.0116	138903.2	143.0062	149607.3	142110.8	143044.6							
3	unknown	15.994	33.0003	7493.109	648218.4	7510.187	539516	7760.35	7785.469	4317.684							
4	unknown	17.0019	4	1634.815	286086.8	1589.771	238737.8	1637.818	1602.784	1022.319							
5	unknown	17.0262	66.0013	1264.488	97.0029	1470.66	79.0019	1491.679	1469.659	3670.108							
6	unknown	18.0352	6504.896	21063.82	1	37557.19	0	43510.67	27598.14	42710.9							
7	unknown	22.9913	455978.5	2084824	40.0005	2032263	26.0002	2120616	2934921	2793823							
8	unknown	23.9843	542.0897	14301.24	743.1685	15212.4	714.1556	15300.22	4710.766	2002.223							
9	unknown	26.0148	3155.036	52026.36	13261.53	53688.11	10396.92	57338.73	52428.99	48788.25							
10	unknown	27.0233	76671.31	536085	908.2517	535729.9	582.1034	593138.2	520893.6	504620.7							
11	unknown	28.0187	5831.365	24001.95	92.0026	21611.92	65.0013	21192.47	25907.76	66699.43							
12	unknown	28.0312	14540.33	68572.17	64.0013	66197.48	48.0007	76905.01	69490.04	74139.43							
13	unknown	29.0028	65847.67	364989.8	1760.946	336658	1187.43	364122.8	349239.1	300321.2							
14	unknown	29.0399	186753.4	374481.2	8	367438.2	4	414047.7	357022.1	346403.8							
15	unknown	29.9981	24515.5	495819	7733.222	476549.3	6426.588	518144.6	490149.9	405782.2							
16	unknown	30.0355	13315.97	34928.69													
17	unknown	31.0189	88250.66	412657.8	1005.												
18	unknown	37.006	472.068	4720.795	1001.												
19	unknown	38.0143	1106.374	20372.13	889.2												
20	unknown	38.9655	28284.75	65280.41													
21	unknown	39.0227	52279.28	320261.5	606.1												
22	unknown	39.9605	794.1925	42016.17													
23	unknown	40.0304	13284.71	56705.06	826.2065	5											
24	unknown	41.0394	258207.4	866719.1	890.2418	8											
25	unknown	42.0103	20659.71	77005.63	21105.35	7											
26	unknown	42.0449	26393.45	102303.5	1908.111	9											
27	unknown	43.0195	123128.9	367378.1	7916.093	3											
28	unknown	43.0552	158256.9	378839.3	975.2902	3											
29	unknown	44.0267	42443.03	111373.1	688.1445	96147.78	526.0845	109688.1	104588.3	111289.6							
30	unknown	44.0514	7462.971	36156.03	96.0028	35960.77	61.0011	37292.21	43857.8	108948.4							
31	unknown	45.0351	110671.1	224522.8	5846.419	187122.2	3801.407	210962.2	199151.9	196157.6							
32	unknown	45.993	142414	1008338	324297.1	911658.3	244863.2	1043108	983091	813230.7							
33	unknown	47.0136	13196	58485.56	1065.346	48603.85	721.1587	54853.07	51021.24	50843.81							
34	unknown	48.0078	958.2802	12777.7	1643.824	11872.92	1251.478	13691.04	12119.72	13252.45							
35	unknown	49.0312	1070.35	2607.073	337.0347	2064.3	248.0188	2521.94	2289.599	2116.366							
36	unknown	50.0135	961.2819	8418.592	529.0854	8698.048	398.0483	8825.729	8843.826	11357.27							
37	unknown	51.0226	4841.145	34527.27	460.0646	33095.01	310.0293	35062.51	32608.35	37066.14							
38	unknown	51.9378	313.0299	14739.1	7	2848.475	0	15467.78	1556.739	10952.53							
39	unknown	52.0303	2967.686	21598.74	253.0195	19658.47	215.0141	21572.4	19343.74	22590.02							
40	unknown	53.0019	14963.12	48000.32	1998.218	41543.26	1376.578	46413.24	54782.76	55099.19							
41	unknown	53.0394	35994.51	135494.3	297.0269	119280.5	190.011	134813.4	116833.4	119638.7							
42	unknown	54.0107	5764.128	31252.18	336.0345	26731.9	246.0185	29849.26	28327.48	29571.27							
43	unknown	54.0461	7119.446	52651	150.0069	47665.69	102.0032	56208.23	46045	50962.44							
44	unknown	55.019	58489.71	236076.8	4876.249	199392.4	3272.266	223120.7	213382.2	266717							
45	unknown	55.0555	82962.45	290683.8	680.1412	273360.4	416.0528	330637.8	259937.4	250321.8							

If this dialog appears, choose 'OK' to save only the active sheet.

The selected file type does not support workbooks that contain multiple sheets.

- To save only the active sheet, click OK.
- To save all sheets, save them individually using a different file name for each, or choose a file type that supports multiple sheets.

OK Cancel



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Ion	Mass	1100_01_1	1100_02_	1100_06_	5100_01_	5100_06_	25100_01_	25500_01_	51000_01_							
2	unknown	15.0236	33461.38	140278.5	195.0116	138903.2	143.0062	149607.3	142110.8	143044.6							
3	unknown	15.994	33.0003	7493.109	648218.4	7510.187	539516	7760.35	7785.469	4317.684							
4	unknown	17.0019	4	1634.815	286086.8	1589.771	238737.8	1637.818	1602.784	1022.319							
5	unknown	17.0262	66.0013	1264.488	97.0029	1470.66	79.0019	1491.679	1469.659	3670.108							
6	unknown	18.0352	6504.896	21063.82	1	37557.19	0	43510.67	27598.14	42710.9							
7	unknown	22.9913	455978.5	2084824	40.0005	2032263	26.0002	2120616	2934921	2793823							
8	unknown	23.9843	542.0897	14301.24	743.1685	15212.4	714.1556	15300.22	4710.766	2002.223							
9	unknown	26.0148	3155.036	52026.36	13261.53	53688.11	10396.92	57338.73	52428.99	48788.25							
10	unknown	27.0233	76671.31	536085	908.2517	535729.9	582.1034	593138.2	520893.6	504620.7							
11	unknown	28.0187	5831.365	24001.95	92.0026	21611.92	65.0013	21192.47	25907.76	66699.43							
12	unknown	28.0312	14540.33	68572.17	64.0013	66197.48	48.0007	76905.01	69490.04	74139.43							
13	unknown	29.0028	65847.67	364989.8	1760.946	336658	1187.43	364122.8	349239.1	300321.2							
14	unknown	29.0399	186753.4	374481.2	8	367438.2	4	414047.7	357022.1	346403.8							
15	unknown	29.9981	24515.5	495819	7733.222	476549.3	6426.588	518144.6	490149.9	405782.2							
16	unknown	30.0355	13315.97	34928.69	8	29409.38	8	29951.1	36942.37	96829.79							
17	unknown	31.0189	88250.66	412657.8	1005.308	374779.1	813.2018	413271.5	389597.1	339247.7							
18	unknown	37.006	472.068	4720.795													
19	unknown	38.0143	1106.374	20372.13													
20	unknown	38.9655	28284.75	65280.41													
21	unknown	39.0227	52279.28	320261.5													
22	unknown	39.9605	794.1925	42016.17													
23	unknown	40.0304	13284.71	56705.06													
24	unknown	41.0394	258207.4	866719.1													
25	unknown	42.0103	20659.71	77005.63	21105.35												
26	unknown	42.0449	26393.45	102303.5	1908.111												
27	unknown	43.0195	123128.9	367378.1	7916.093												
28	unknown	43.0552	158256.9	378839.3	975.2902												
29	unknown	44.0267	42443.03	111373.1	688.1445	96147.76	528.0645	109666.1	104566.3	111263.6							
30	unknown	44.0514	7462.971	36156.03	96.0028	35960.77	61.0011	37292.21	43857.8	108948.4							
31	unknown	45.0351	110671.1	224522.8	5846.419	187122.2	3801.407	210962.2	199151.9	196157.6							
32	unknown	45.993	142414	1008338	324297.1	911658.3	244863.2	1043108	983091	813230.7							
33	unknown	47.0136	13196	58485.56	1065.346	48603.85	721.1587	54853.07	51021.24	50843.81							
34	unknown	48.0078	958.2802	12777.7	1643.824	11872.92	1251.478	13691.04	12119.72	13252.45							
35	unknown	49.0312	1070.35	2607.073	337.0347	2064.3	248.0188	2521.94	2289.599	2116.366							
36	unknown	50.0135	961.2819	8418.592	529.0854	8698.048	398.0483	8825.729	8843.826	11357.27							
37	unknown	51.0226	4841.145	34527.27	460.0646	33095.01	310.0293	35062.51	32608.35	37066.14							
38	unknown	51.9378	313.0299	14739.1	7	2848.475	0	15467.78	1556.739	10952.53							
39	unknown	52.0303	2967.686	21598.74	253.0195	19658.47	215.0141	21572.4	19343.74	22590.02							
40	unknown	53.0019	14963.12	48000.32	1998.218	41543.26	1376.578	46413.24	54782.76	55099.19							
41	unknown	53.0394	35994.51	135494.3	297.0269	119280.5	190.011	134813.4	116833.4	119638.7							
42	unknown	54.0107	5764.128	31252.18	336.0345	26731.9	246.0185	29849.26	28327.48	29571.27							
43	unknown	54.0461	7119.446	52651	150.0069	47665.69	102.0032	56208.23	46045	50962.44							
44	unknown	55.019	58489.71	236076.8	4876.249	199392.4	3272.266	223120.7	213382.2	266717							
45	unknown	55.0555	82962.45	290683.8	680.1412	273360.4	416.0528	330637.8	259937.4	250321.8							

If this dialog appears, choose 'Yes' to keep the current format.

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 copy in the latest Excel format.
- To see what might be lost, click Help.

Yes No Help

	A	B	C
1	Ion	Mass	1100_01_
2	unknown	15.0236	33461.38
3	unknown	15.994	33.0003
4	unknown	17.0019	
5	unknown	17.0262	66.0013
6	unknown	18.0352	6504.898
7	unknown	22.9913	455978.8
8	unknown	23.9843	542.0897
9	unknown	26.0148	3155.038
10	unknown	27.0233	76671.31
11	unknown	28.0187	5831.368
12	unknown	28.0312	14540.33
13	unknown	29.0028	65847.67
14	unknown	29.0399	186753.4
15	unknown	29.9981	24515.8
16	unknown	30.0355	13315.97
17	unknown	31.0189	88250.68
18	unknown	37.006	472.068
19	unknown	38.0143	1106.374
20	unknown	38.9655	28284.78
21	unknown	39.0227	52279.28
22	unknown	39.9605	794.1928
23	unknown	40.0304	13284.71
24	unknown	41.0394	258207.4
25	unknown	42.0103	20659.71
26	unknown	42.0449	26393.48
27	unknown	43.0195	123128.9
28	unknown	43.0552	158256.9
29	unknown	44.0267	42443.03
30	unknown	44.0514	7462.971
31	unknown	45.0351	110671.1
32	unknown	45.993	142414
33	unknown	47.0136	13198
34	unknown	48.0078	958.2802
35	unknown	49.0312	1070.38
36	unknown	50.0135	961.2819
37	unknown	51.0226	4841.148
38	unknown	51.9378	313.0298
39	unknown	52.0303	2967.688
40	unknown	53.0019	14963.12
41	unknown	53.0394	35994.51
42	unknown	54.0107	5764.128
43	unknown	54.0461	7119.448
44	unknown	55.019	58489.71
45	unknown	55.0555	82962.48

fortutorial

File Edit View Favorites Tools Help

Back Search Folders

Address C:\fortutorial Go

Name	Size	Type	Date Modified
1100_01_1.ITS	1,366 KB	TOF-SIMS Spectrum	10/4/2010 12:56 PM
1100_02_.ITS	1,432 KB	TOF-SIMS Spectrum	10/4/2010 12:56 PM
1100_06_.ITS	930 KB	TOF-SIMS Spectrum	10/1/2010 4:01 PM
5100_01_.ITS	1,382 KB	TOF-SIMS Spectrum	10/4/2010 12:56 PM
5100_06_.ITS	832 KB	TOF-SIMS Spectrum	10/1/2010 4:01 PM
25100_01_.ITS	1,409 KB	TOF-SIMS Spectrum	10/4/2010 12:56 PM
25500_01_.ITS	1,375 KB	TOF-SIMS Spectrum	10/4/2010 12:56 PM
51000_01_.ITS	1,420 KB	TOF-SIMS Spectrum	10/1/2010 4:52 PM
posnew.itmil			
v6fortutorial.txt			

Folders

- Desktop
- My Documents
- My Computer
  - Local Disk (C:)
    - Acrobat Reader
    - ATI
    - bif
    - cabs
    - data
    - dell
    - Documents and Settings
    - eaf4236bcb169392585085
    - foo
    - fortutorial
    - frames
    - Intel
    - lj4100-4100mfp
    - Manuals
    - MyStuff
      - Admin
      - Conferences
      - Drupal
      - info
      - Instruments
      - nb\_tools\_v1.0
      - NBScripts
      - NBStuff
      - NewCodeIdeas
      - OthersCode
      - Papers
      - PapersToReview
      - SARC
      - Software
      - Teaching
      - testingfiles
      - WorkingData
        - AminoAcids
        - BethSIMS
        - DataToTake
        - foo
        - JeremyRaxton2010\_00

If the file you saved is not in the active Matlab folder, then make a copy and put it in the active Matlab folder.

	A	B	C
1	Ion	Mass	1100_01
2	unknown	15.0236	33461.38
3	unknown	15.994	33.0003
4	unknown	17.0019	
5	unknown	17.0262	66.0013
6	unknown	18.0352	6504.896
7	unknown	22.9913	455978.8
8	unknown	23.9843	542.0897
9	unknown	26.0148	3155.036
10	unknown	27.0233	76671.31
11	unknown	28.0187	5831.368
12	unknown	28.0312	14540.33
13	unknown	29.0028	65847.67
14	unknown	29.0399	186753.4
15	unknown	29.9981	24515.8
16	unknown	30.0355	13315.97
17	unknown	31.0189	88250.68
18	unknown	37.006	472.068
19	unknown	38.0143	1106.374
20	unknown	38.9655	28284.78
21	unknown	39.0227	52279.28
22	unknown	39.9605	794.1928
23	unknown	40.0304	13284.71
24	unknown	41.0394	258207.4
25	unknown	42.0103	20659.71
26	unknown	42.0449	26393.48
27	unknown	43.0195	123128.9
28	unknown	43.0552	158256.9
29	unknown	44.0267	42443.03
30	unknown	44.0514	7462.971
31	unknown	45.0351	110671.1
32	unknown	45.993	142414
33	unknown	47.0136	13198
34	unknown	48.0078	958.2802
35	unknown	49.0312	1070.38
36	unknown	50.0135	961.2819
37	unknown	51.0226	4841.148
38	unknown	51.9378	313.0298
39	unknown	52.0303	2967.688
40	unknown	53.0019	14963.12
41	unknown	53.0394	35994.51
42	unknown	54.0107	5764.128
43	unknown	54.0461	7119.448
44	unknown	55.019	58489.71
45	unknown	55.0555	82962.48

work

File Edit View Favorites Tools Help

Address  Go

Name	Size	Type	Date Modified
25500_01.BIF6	38,403 KB	BIF6 File	10/4/2010 12:42
25100_01.BIF6	38,403 KB	BIF6 File	10/4/2010 12:34
5100_06.BIF6	13,313 KB	BIF6 File	10/4/2010 1:34 P
5100_01.BIF6	38,403 KB	BIF6 File	10/4/2010 12:49
1100_06.BIF6	13,313 KB	BIF6 File	10/4/2010 1:28 P
1100_02.BIF6	38,403 KB	BIF6 File	10/4/2010 12:16
TIMAGE.BIF	8,580 KB	BIF File	4/29/2010 2:15 P
TESTP04.bif	77,961 KB	BIF File	7/16/2010 7:57 P
S1200_03.BIF	10,114 KB	BIF File	9/9/2010 3:53 P
S1200_01.BIF	10,114 KB	BIF File	9/9/2010 3:47 P
S103.BIF	3,202 KB	BIF File	3/18/2010 4:57 P
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 P
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 P
S2GL_08.BIF	12,290 KB	BIF File	9/9/2010 4:04 P
S2GL_07.BIF	10,114 KB	BIF File	9/9/2010 3:34 P
S2GL_06.BIF	5,443 KB	BIF File	9/8/2010 1:38 P
S2GL_05.BIF	2,946 KB	BIF File	9/8/2010 2:57 P
S1GL_06.BIF	21,763 KB	BIF File	9/8/2010 1:42 P
S1GL_05.BIF	10,114 KB	BIF File	9/9/2010 3:43 P
S1GL_04.BIF	12,290 KB	BIF File	9/9/2010 4:06 P
S1_02.BIF	7,492 KB	BIF File	3/2/2010 3:31 P
NA2100_2.BIF	112,012 KB	BIF File	1/4/2010 4:48 P
MT1_5.BIF	18,050 KB	BIF File	7/8/2010 1:24 P
J1N.BIF	3,841 KB	BIF File	9/2/2010 10:41 P
F1N.BIF	3,841 KB	BIF File	9/2/2010 10:41 P
DAN01.BIF	2,817 KB	BIF File	1/4/2010 4:48 P
D4.BIF	4,097 KB	BIF File	9/2/2010 10:24 P
	4,097 KB	BIF File	9/2/2010 10:24 P
	16,898 KB	BIF File	5/11/2010 9:00 P
	3,841 KB	BIF File	9/2/2010 10:24 P
	3,841 KB	BIF File	9/2/2010 10:40 P
	4,097 KB	BIF File	9/2/2010 10:23 P
3D_NEG.	2,945 KB	BIF File	6/28/2010 12:17
1TEST.B	18,434 KB	BIF File	3/10/2010 12:18
codeforzoffsetsfg.asv	2 KB	ASV File	7/28/2010 2:24 P
v6fortutorial.txt	15 KB	Text Document	10/11/2010 3:39

Once the file is in the active Matlab folder, you are ready to import it into the spectragui.

MATLAB 7.3.0 (R2006b)

File Edit Debug Desktop Window Help

Shortcuts How to Add What's New

Workspace

Name

Current Directory

Command History

```
8/13/10 9:4
spectragui
```

spectragui

File Data Pre-Processing MVA Data Display

Section Panel

in further analysis unless you specify otherwise

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

Select Data Select Totalcounts Select Samples

← →

Now lets load some data.

From the Data Pre-Processing menu choose ->Import Data ->Iontof



**Workspace**

Name

Current Directory

**Command History**

```

>> spectragui
  
```

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

Now lets load some data.

From the Data Pre-Processing menu choose ->Import Data ->Iontof

these are the main input data that you can use to load data

Name of Variable Matrix:

Name of Variable Matrix:

Name of Variable Matrix:

Name of Samplenames Matrix:

### 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="Select Samples"/>

Use the buttons below to import an excel file or a tab delimited text file that has been exported directly from the iontof software.

Use the dialog box on the right to import data using the old import format with the modified text file.

Legacy IonTof Data import

Name of .txt. file

Number of Files in Data Set

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

Enter the number of files in the data set in the box below.



### 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	Select Samples

Use the buttons below to import an excel file or a tab delimited text file that has been exported directly from the iontof software.

Use the dialog box on the right to import data using the old import format with the modified text file.

Import Excel

Import TXT

Legacy IonTof Data import

Name of .txt. file

newcIn.txt

Number of Files in Data Set

42

Import Data

Close Panel

Press the 'Import Data' button and the data is read into the Matlab workspace and into the spectragui

← →



### 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	Select Samples

Use the buttons below to import an excel file or a tab delimited text file that has been exported directly from the iontof software.

Use the dialog box on the right to import data using the old import format with the modified text file.

Import Excel

Import TXT

#### Legacy IonTof Data import

Name of .txt. file

newcln.txt

Number of Files in Data Set

42

Import Data

Close Panel

The data is loaded and placed in the respective drop down 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

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

Here we will look at how to import lntof peak area data from an excel spreadsheet.





Check...

Add Peak

Mass (u)

Dev. (ppm)

?

Area (cts)

Counts / Shot

Resolution

Width (ns)

erties

### Peak Statistics

Icons: Save, Print, Filter, Sort, etc. | Labels: Mean, SD, RSD, ΣI

Peak Label	Mass	GTP_614_HM...	GTP_614_HM...	GTP_614_HM...	GTP_614_HM...	GTP_614_HM...	GTP_614_HM...	GTP_614_HM...	GTP_614_HM...	GTP_614_HM...
	22.9892	36937.71	183823.18	232332.18	457335.31	301314.74	310307.38	1306139.08	643860.22	285359
	29.0014	29820.92	44868.97	49108.12	46250.81	52748.52	145959.29	156603.81	172762.51	137068
	29.0386	818183.65	1339621.39	1388887.14	1663618.39	1613987.57	3846666.22	2586341.05	2341713.36	4239610
	41.0375	1497060.60	2530065.82	2592362.09	3115099.68	3083298.51	5954584.58	4014577.11	3655666.23	6503085
	57.0727	1197650.79	1922459.67	1912262.31	2540560.04	2378313.30	2617528.02	1550213.91	1389797.21	2937113
	69.0728	521575.97	835238.97	848543.97	1135566.26	1039861.52	970769.21	564580.30	495464.86	1054171
	71.0946	468991.18	729111.12	732785.07	1024871.06	897767.17	890860.88	508834.72	446994.20	1009072
	164.9183	3606.89	3882.12	3692.87	5167.01	4438.00	6844.63	16191.86	19646.23	7267
TotalCounts		21937689	31763506	32742573	40074036	38256610	61484102	48715049	45689098	66947

**Statistic Data List Layout Option**

Print Precision:  
Mass: 4  
Others: 2

Description:  
 Assignment  
 Mass  
 Description

Cancel OK

Make sure the Description field is 'Mass'

← →



File Home Menu Insert Page Layout Formulas Data Review View Team

Clipboard: Cut, Copy, Paste, Format Painter

Font: Calibri, 11, Bold, Italic, Underline, Text Color, Background Color

Alignment: Wrap Text, Merge & Center

Number: General, Currency, Percentage, Decimals

Styles: Conditional Formatting, Format as Table, Cell Styles

Cells: Insert, Delete

A1 fx Date : 10.08.2013

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	Date	: 10.08.2013														
2	Time	: 10:28:52														
3	File(s)	: GTP_614_HMR_01_0														
4		GTP_614_HMR_02_0														
5		GTP_614_HMR_03_0														
6		GTP_614_HMR_04_0														
7		GTP_614_HMR_05_0														
8		GTP_614_HMRC60_01_0														
9		GTP_614_HMRC60_02_0														
10		GTP_614_HMRC60_03_0														
11		GTP_614_HMRC60_04_0														
12		GTP_614_HMRC60_05_0														
13	Peak Label	Mass	Spectra:	Corrected Area:												
14			GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614_HMRC60_05_0
15		22.9892	36937.71	183823.2	232332.2	457335.3	301314.7	310307.4	1306139	643860.2	285359.7	735715.1				
16		29.0014	29820.92	44868.97	49108.12	46250.81	52748.52	145959.3	156603.8	172762.5	137068.6	154939.1				
17		29.0386	818183.7	1339621	1388887	1663618	1613988	3846666	2586341	2341713	4239611	3133547				
18		41.0375	1497061	2530066	2592362	3115100	3083299	5954585	4014577	3655666	6503086	4842988				
19		57.0727	1197651	1922460	1912262	2540560	2378313	2617528	1550214	1389797	2937114	2027455				
20		69.0728	521576	835239	848544	1135566	1039862	970769.2	564580.3	495464.9	1054172	728484.9				
21		71.0946	468991.2	729111.1	732785.1	1024871	897767.2	890860.9	508834.7	446994.2	1009073	679331.1				
22		164.9183	3606.89	3882.12	3692.87	5167.01	4438	6844.63	16191.86	19646.23	7267.83	14583.41				
23	TotalCounts		21937689	31763506	32742573	40074036	38256610	61484102	48715049	45689098	66947965	54165464				

Then paste the data into Excel.

(Ctrl) Paste Options:

Keep Text Only (T)

File Home Menu Insert Page Layout Formulas Data Review View Team

Clipboard: Paste, Cut, Copy, Format Painter

Font: Calibri, 11, Bold, Italic, Underline, Text Color, Background Color

Alignment: Wrap Text, Merge & Center

Number: General, \$, %, , , .00, .0

Styles: Conditional Formatting, Format as Table, Cell Styles

Cells: Insert, Delete

B15 fx

A B C D E F G H I J K L M N O P

1	Date	: 10.08.2013														
2	Time	: 10:28:52														
3	File(s)	: GTP_614_HMR_01_0														
4		GTP_614_HMR_02_0														
5		GTP_614_HMR_03_0														
6		GTP_614_HMR_04_0														
7		GTP_614_HMR_05_0														
8		GTP_614_HMRC60_01_0														
9		GTP_614_HMRC60_02_0														
10		GTP_614_HMRC60_03_0														
11		GTP_614_HMRC60_04_0														
12		GTP_614_HMRC60_05_0														

13	Peak Label	Mass	Spectra:	Corrected Area:											
14				GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614_HMRC60_05_0
15	22.9892		36937.71	183823.2	232332.2	457335.3	301314.7	310307.4	1306139	643860.2	285359.7	735715.1			
16	29.0014		2						5959.3	156603.8	172762.5	137068.6	154939.1		
17	29.0386		2						846666	2586341	2341713	4239611	3133547		
18	41.0375		1						954585	4014577	3655666	6503086	4842988		
19	57.0727		1						617528	1550214	1389797	2937114	2027455		
20	69.0728		1						0769.2	564580.3	495464.9	1054172	728484.9		
21	71.0946		4						0860.9	508834.7	446994.2	1009073	679331.1		
22	164.9183		3606.89	3882.12	3692.87	5167.01	4438	6844.63	16191.86	19646.23	7267.83	14583.41			
23	TotalCounts		21937689	31763506	32742573	40074036	38256610	61484102	48715049	45689098	66947965	54165464			

Move the mass labels over to the first column





Check...

Add Peak

Mass (u)

Dev. (ppm)

?

Area (cts)

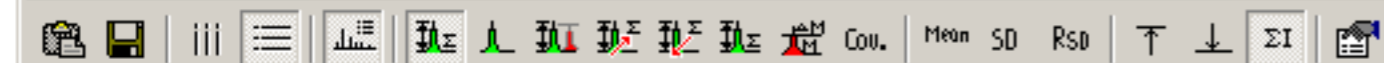
Counts / Shot

Resolution

Width (ns)

erties

### Peak Statistics



Peak Label	Mass	GTP_614_HM...	GTP_614_HM...	GTP_614_HM...	GTP_614_HM...	GTP_614_HM...	GTP_614_HM...	GTP_614_HM...	GTP_614_HM...	GTP_614_HM...
	22.9892	36937.71	183823.18	232332.18	457335.31	301314.74	310307.38	1306139.08	643860.22	285359
	29.0014	29820.92	44868.97	49108.12	46250.81	52748.52	145959.29	156603.81	172762.51	137068
	29.0386	818183.65	1339621.39	1388887.14	1663618.39	1613987.57	3846666.22	2586341.05	2341713.36	4239610
	41.0375	1497060.60	2530065.82	2592362.09	3115099.68	3083298.51	5954584.58	4014577.11	3655666.23	6503085
	57.0727	1197650.79	1922459.67	1912262.31	2540560.04	2378313.30	2617528.02	1550213.91	1389797.21	2937113
	69.0728	521575.97	835238.97	848543.97	1135566.26	1039861.52	970769.21	564580.30	495464.86	1054171
	71.0946	468991.18	729111.12	732785.07	1024871.06	897767.17	890860.88	508834.72	446994.20	1009072
	164.9183	3606.89	3882.12	3692.87	5167.01	4438.00	6844.63	16191.86	19646.23	7267
TotalCounts		21937689	31763506	32742573	40074036	38256610	61484102	48715049	45689098	669479

**Statistic Data List Layout Option** [X]

Print Precision:

Mass:

Others:

Description:

Assignment

Mass

Description

Cancel OK

Now change the Description to 'Description'.

← →



Check...

Add Peak

Mass (u)

Dev. (ppm)

?

Area (cts)

Counts / Shot

Resolution

Width (ns)

erties

Peak Statistics

Press the copy button.

Peak Label	GTP_614_HM...	GTP_614_HM...	GTP_614_HM...	GTP_614_HM...	GTP_614_HM...	GTP_614_HM...	GTP_614_HM...		
	232332.18	457335.31	301314.74	310307.38	1306139.08	643860.22	285359		
	49108.12	46250.81	52748.52	145959.29	156603.81	172762.51	137068		
	1388887.14	1663618.39	1613987.57	3846666.22	2586341.05	2341713.36	4239610		
C3H5	1497060.60	2530065.82	2592362.09	3115099.68	3083298.51	5954584.58	4014577.11	3655666.23	6503085
C4H9	1197650.79	1922459.67	1912262.31	2540560.04	2378313.30	2617528.02	1550213.91	1389797.21	2937113
C5H9	521575.97	835238.97	848543.97	1135566.26	1039861.52	970769.21	564580.30	495464.86	1054171
C5H11	468991.18	729111.12	732785.07	1024871.06	897767.17	890860.88	508834.72	446994.20	1009072
unknown	3606.89	3882.12	3692.87	5167.01	4438.00	6844.63	16191.86	19646.23	7267
TotalCounts	21937689	31763506	32742573	40074036	38256610	61484102	48715049	45689098	66947

File Home Menu Insert Page Layout Formulas Data Review View Team

Clipboard: Paste, Cut, Copy, Format Painter

Font: Calibri, 11, Bold, Italic, Underline, Text Color, Background Color

Alignment: Wrap Text, Merge & Center

Number: General, \$, %, , , .00, .00

Styles: Conditional Formatting, Format as Table, Cell Styles

Cells: Insert, Delete

B15 fx Na

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	Date	: 10.08.2013														
2	Time	: 10:29:16														
3	File(s)	: GTP_614_HMR_01_0														
4		GTP_614_HMR_02_0														
5		GTP_614_HMR_03_0														
6		GTP_614_HMR_04_0														
7		GTP_614_HMR_05_0														
8		GTP_614_HMRC60_01_0														
9		GTP_614_HMRC60_02_0														
10		GTP_614_HMRC60_03_0														
11		GTP_614_HMRC60_04_0														
12		GTP_614_HMRC60_05_0														
13	Peak Label	Mass	Spectra:	Corrected Area:												
14			GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614	GTP_614_HMRC60_05_0
15	Na	36937.71	183823.2	232332.2	457335.3	301314.7	310307.4	1306139	643860.2	285359.7	735715.1					
16	CHO	29820.9						156603.8	172762.5	137068.6	154939.1					
17	C2H5							2586341	2341713	4239611	3133547					
18	C3H5	149706						4014577	3655666	6503086	4842988					
19	C4H9	119765						1550214	1389797	2937114	2027455					
20	C5H9	52157						564580.3	495464.9	1054172	728484.9					
21	C5H11	468991						508834.7	446994.2	1009073	679331.1					
22	unknown	3606.89	3882.12	3692.87	5167.01	4438	6844.63	16191.86	19646.23	7267.83	14583.41					
23	TotalCounts	21937689	31763506	32742573	40074036	38256610	61484102	48715049	45689098	66947965	54165464					
24																
25																
26																
27																
28																
29																
30																
31																
32																
33																
34																
35																

Then paste the data into Excel onto a separate sheet. Copy the labels.

(Ctrl)



File Home Menu Insert Page Layout Formulas Data Review View Team

Clipboard: Paste, Cut, Copy, Format Painter

Font: Calibri, 11, Bold, Italic, Underline, Text Color, Background Color

Alignment: Wrap Text, Merge & Center, Left, Center, Right, Indent, Decrease Indent, Increase Indent

Number: General, Currency, Percentage, Decimals, Thousands Separator

Styles: Conditional Formatting, Format as Table, Cell Styles

Cells: Insert, Delete

B15 fx

A B C D E F G H I J K L M N O P

1	Date	: 10.08.2013														
2	Time	: 10:28:52														
3	File(s)	: GTP_614_HMR_01_0														
4		GTP_614_HMR_02_0														
5		GTP_614_HMR_03_0														
6		GTP_614_HMR_04_0														
7		GTP_614_HMR_05_0														
8		GTP_614_HMRC60_01_0														
9		GTP_614_HMRC60_02_0														
10		GTP_614_HMRC60_03_0														
11		GTP_614_HMRC60_04_0														
12		GTP_614_HMRC60_05_0														

13	Peak Label	Mass	Spectra:	Corrected Area:													
14			GTP_614					GTP_614	GTP_614	GTP_614	GTP_614	HMRC60_05_0					
15	22.9892							1306139	643860.2	285359.7	735715.1						
16	29.0014							156603.8	172762.5	137068.6	154939.1						
17	29.0386							2586341	2341713	4239611	3133547						
18	41.0375							4014577	3655666	6503086	4842988						
19	57.0727							1550214	1389797	2937114	2027455						
20	69.0728			521576	835239	848544	1135566	1039862	970769.2	564580.3	495464.9	1054172	728484.9				
21	71.0946			468991.2	729111.1	732785.1	1024871	897767.2	890860.9	508834.7	446994.2	1009073	679331.1				
22	164.9183			3606.89	3882.12	3692.87	5167.01	4438	6844.63	16191.86	19646.23	7267.83	14583.41				
23	TotalCounts			21937689	31763506	32742573	40074036	38256610	61484102	48715049	45689098	66947965	54165464				

Then paste them into this column.



spectragui

File Data Pre-Processing MVA Data Display

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

These are the main input data. Specify otherwise.  
Use the drop down menus to select your analysis.

Name of Variable Matrix      Name of Counts Matrix      Name of Samplenames Matrix

Select Data      Select Variables      Select Filenames      Select Totalcounts      Select Samples

Choose 'Iontof' from the 'Data Pre-Processing' -> 'Import Data' 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	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="Select Samples"/>

Use the buttons below to import an excel file or a tab delimited text file that has been exported directly from the iontof softare.

Use the dialog box on the right to import data using the old import format with the modified text file.

Legacy IonTof Data import

Name of .txt. file

Number of Files in Data Set

Import Data

Import Excel

Import TXT

Press the 'Import Excel' button.

← →

Close Panel



spectragui

Pick a file

Look in: MATLAB

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		
TestSpreadsheetImportFile.xlsx	10/8/2013 10:31 AM	Microsoft Excel ...	12 KB	
~\$TestSpreadsheetImportFile.xlsx	10/8/2013 10:30 AM	Microsoft Excel ...	1 KB	
NegIonData_MS.xlsx	8/21/2013 1:19 PM	Microsoft Excel ...	42 KB	
AllPosData.xlsx	8/20/2013 4:02 PM	Microsoft Excel ...	172 KB	
PSPEGROI.xlsx	7/2/2013 2:47 PM	Microsoft Excel ...	22 KB	
MDXWT Pos Master All PREVIOUS EXP Included.xlsx	2/12/2013 3:57 PM	Microsoft Excel ...	1,078 KB	
Computer - Shortcut	2/6/2013 9:58 AM	Shortcut	1 KB	
Shortneglist.xlsx	11/7/2012 4:27 PM	Microsoft Excel ...	13 KB	
spectracoparisonneg.xlsx	10/23/2012 4:15 PM	Microsoft Excel ...	14 KB	
dpcomp148con.xlsx	10/23/2012 3:59 PM	Microsoft Excel ...	10 KB	

File name: TestSpreadsheetImportFile.xlsx

Files of type: new xcel files (\*.xlsx)

Open

Cancel

Select the file and press 'Open'.



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="Select Samples"/>

Use the buttons below to import an excel file or a tab delimited text file that has been exported directly from the iontof software.

Use the dialog box on the right to import data using the old import format with the modified text file.

#### Legacy IonTof Data import

Name of .txt. file

Number of Files in Data Set

The data is imported and populated into the respective drop down menus in the 'Data Selection 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="Select Samples"/>

Use the buttons below to import an excel file or a tab delimited text file that has been exported directly from the iontof softare.

Use the dialog box on the right to import data using the old import format with the modified text file.

Legacy IonTof Data import

Name of .txt. file

Number of Files in Data Set

You can then close the panel.



**Workspace**

Name

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

Current Directory

**Command History**

```

>> spectragui
  
```

### Raw Data Selection Panel

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

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

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.

←      →

