To Plot a Graph in Origin

Example: Number of Counts from a Geiger-Müller Tube as a Function of Supply Voltage

Digression on Error Bars

- What entity do you use for the magnitude of the error bars?
- Standard Deviation
  - Assumes data are “normally distributed”
  - A given measurement has a 68% probability of falling within σ of the mean of the measurements
  - It has a 95.5% probability of falling within 2xσ.
  - Standard deviation only gives information about how close to the mean any given measurement can be expected to be.
  - Value of standard deviation depends little on number of measurements
  - Standard deviation is not useful for generating error bars.

Error Bars

- Standard Deviation of the Mean (SDoM)
  - Aka “Standard Error of the Mean”
  - Refers to the distribution of means (averages) of a series of measurements about the population mean.
    - Remember that the population mean is what you get by taking a census of all members of the population
  - There is a 68% probability that the mean of your measurements lies within one standard deviation of the mean of the true mean of the entire population. Get that?
- Good news: Mean of measurements approaches population mean with increasing number of measurements
- Bad news: Only approaches as $1/\sqrt{N}$
- SDoM approaches zero with increasing number of measurements

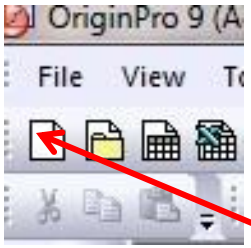
Error Bars

- The entity you want to plot as error bars is the Standard Deviation of the Mean ("Standard Error" for Origin).
  - Excel will calculate the Standard Deviation of a series of data/measurements
  - Excel will also determine the number of measurements
    - Rarely useful
    - How would you not know how many data you took?
    - Not equal to number of rows of data in Excel?
  - SDoM = SD/SQRT(N)

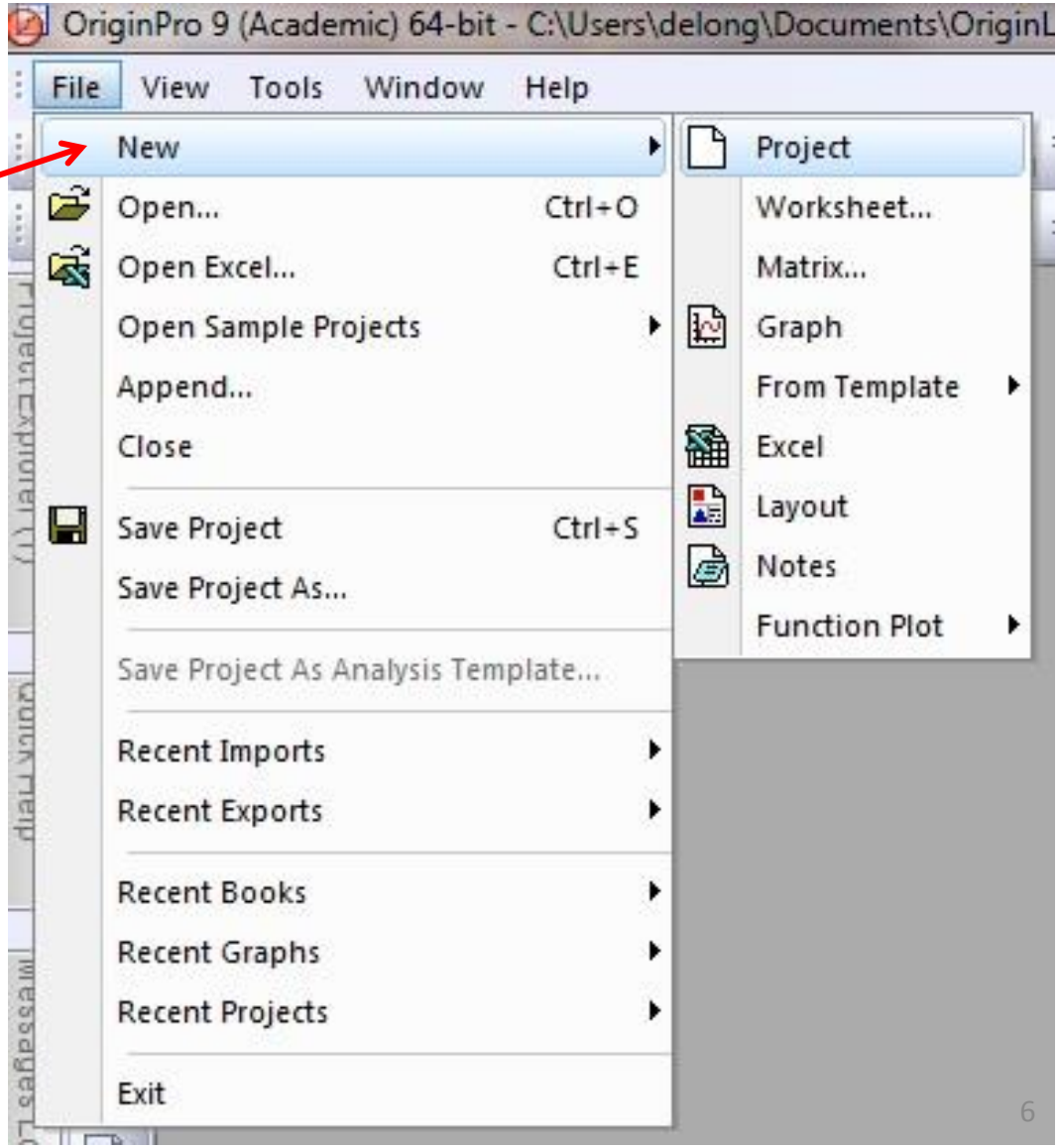
Back to Plotting in Origin with Error Bars

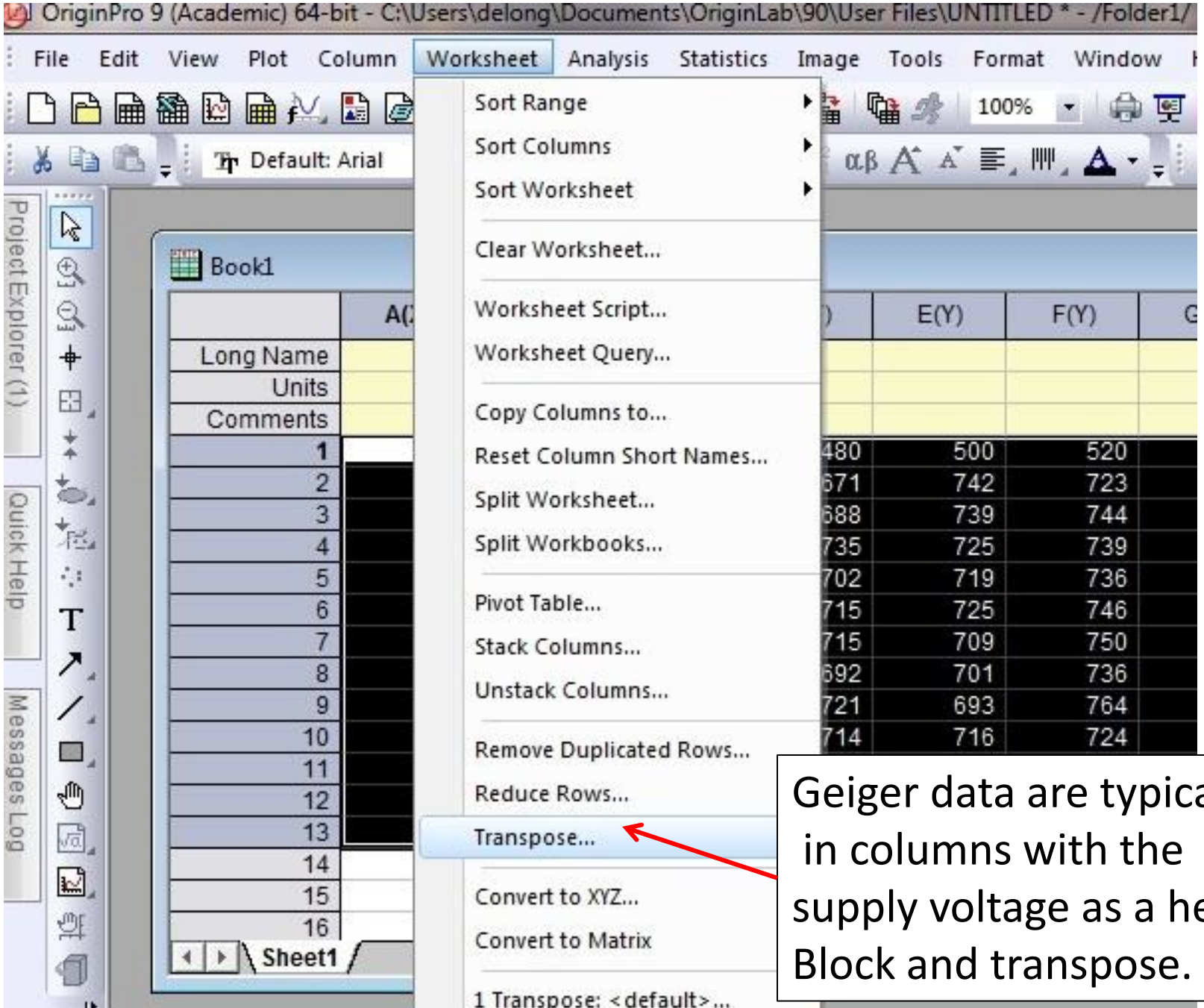
- File:New or the New Project icon (next slide)
- Enter data (two slides down)
  - Manually (e.g. Pendulum)
  - Copy and paste
  - From Excel…
  - Data

Getting Started in Origin



New project





Geiger data are typically in columns with the supply voltage as a header. Block and transpose.

Plotting in Origin, cont'd

- Data to be plotted horizontally ("independent variable") must be in first column set as X or you may use another column set as Y and change it to X
- Data to be plotted vertically ("dependent variable", typically multiple measurements thereof) must be in columns to right of x-values
- If initial format is opposite (e.g. Geiger data)
  - Worksheet:Transpose: Open Dialog:Ok (two slides down)

Format for generating mean, SD and SDoM

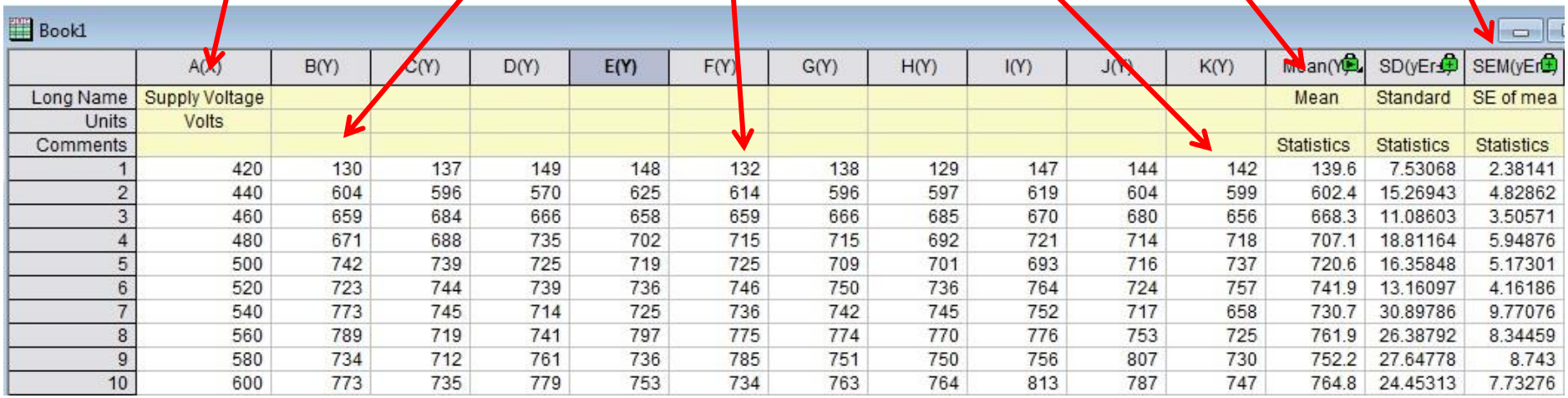
- Block all (only) data for statistical analysis…click and drag…like blocking in any program?
- Statistics:Descriptive statistics:Statistics on rows (or “on columns” if your data are displayed in that way) :Open dialog
  - De-select everything, specifically including the “Optional Report” and “Quartiles”, except Mean, SD and (add) Standard Error of Mean.
- Ok
- Mean, Standard Deviation and Standard Error of Mean will appear in columns to the right of data or in a new sheet

"Independent variable" values

Multiple values of dependent variable

Mean

SDoM

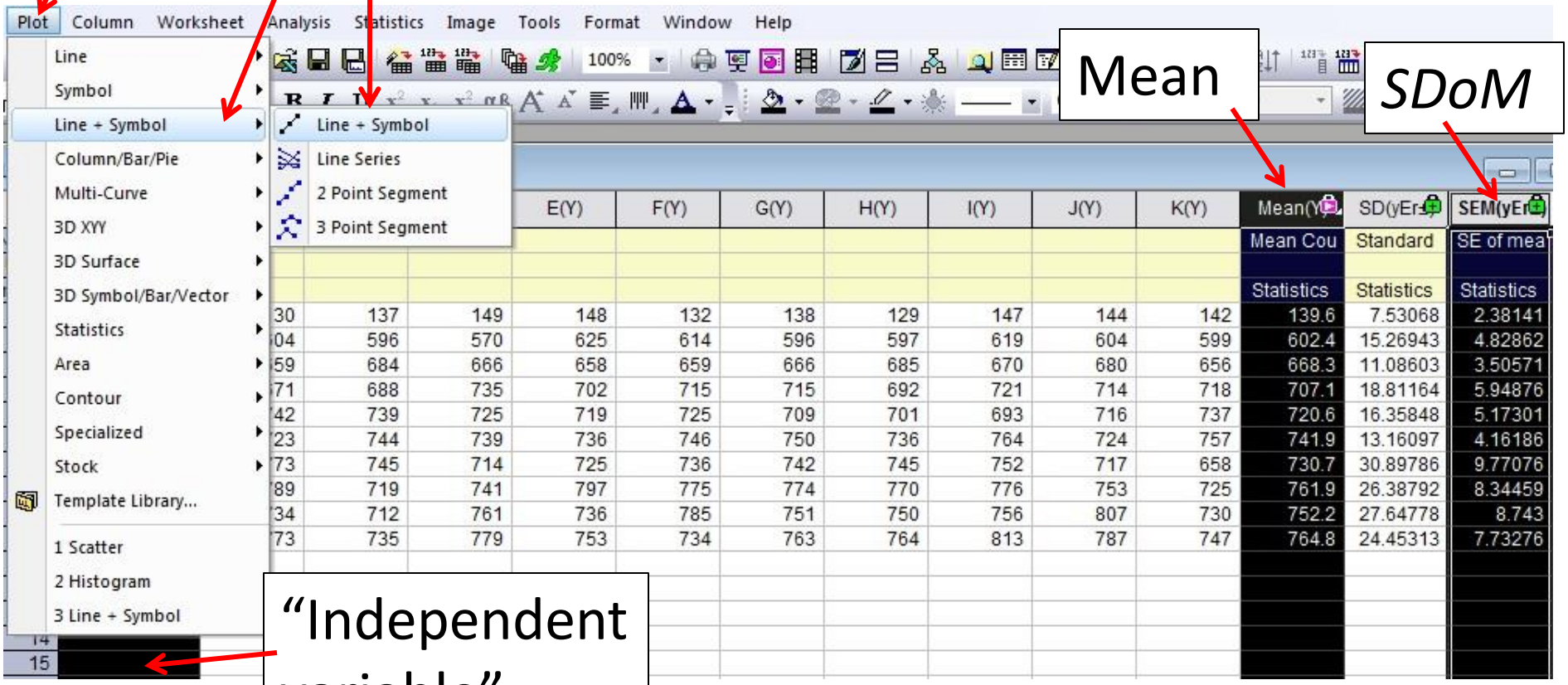


Book1

	A(X)	B(Y)	C(Y)	D(Y)	E(Y)	F(Y)	G(Y)	H(Y)	I(Y)	J(Y)	K(Y)	Mean(Y)	SD(yEr)	SEM(yEr)
Long Name	Supply Voltage											Mean	Standard	SE of mea
Units	Volts													
Comments												Statistics	Statistics	Statistics
1	420	130	137	149	148	132	138	129	147	144	142	139.6	7.53068	2.38141
2	440	604	596	570	625	614	596	597	619	604	599	602.4	15.26943	4.82862
3	460	659	684	666	658	659	666	685	670	680	656	668.3	11.08603	3.50571
4	480	671	688	735	702	715	715	692	721	714	718	707.1	18.81164	5.94876
5	500	742	739	725	719	725	709	701	693	716	737	720.6	16.35848	5.17301
6	520	723	744	739	736	746	750	736	764	724	757	741.9	13.16097	4.16186
7	540	773	745	714	725	736	742	745	752	717	658	730.7	30.89786	9.77076
8	560	789	719	741	797	775	774	770	776	753	725	761.9	26.38792	8.34459
9	580	734	712	761	736	785	751	750	756	807	730	752.2	27.64778	8.743
10	600	773	735	779	753	734	763	764	813	787	747	764.8	24.45313	7.73276

Plot

Line + Symbol



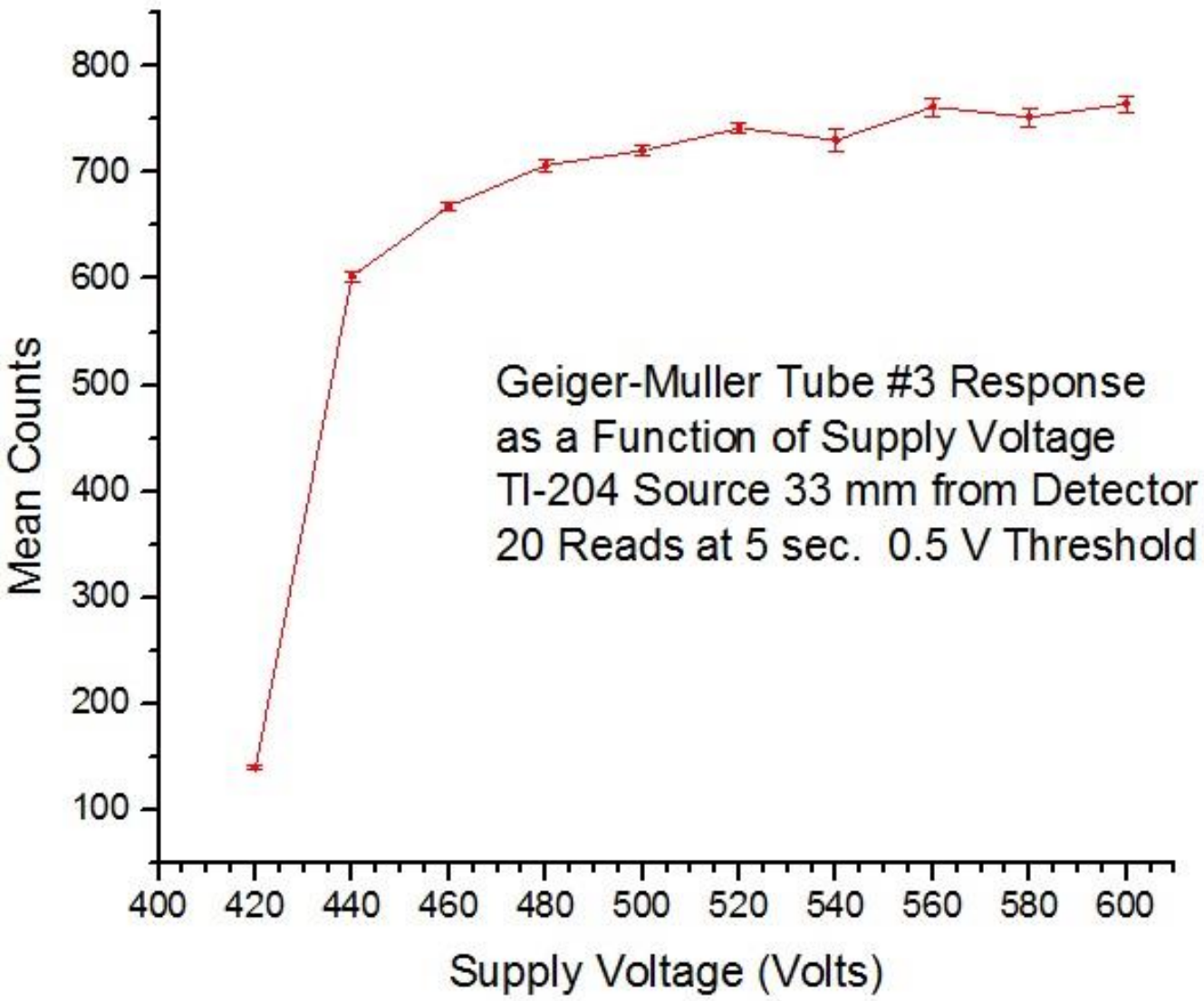
Mean

SDoM

"Independent variable" values

- Block the first column [A(x)], [CTRL: click above column] the third from last [Mean] and last [SE of Mean] columns
- Plot:Line:Scatter
- If you double click on the plot (line or point) a menu appears allowing you to choose line and line+symbol curve, line or symbol shape, size and color, etc.
  - If your data are any good you will have to choose much smaller symbols to see your error bars!

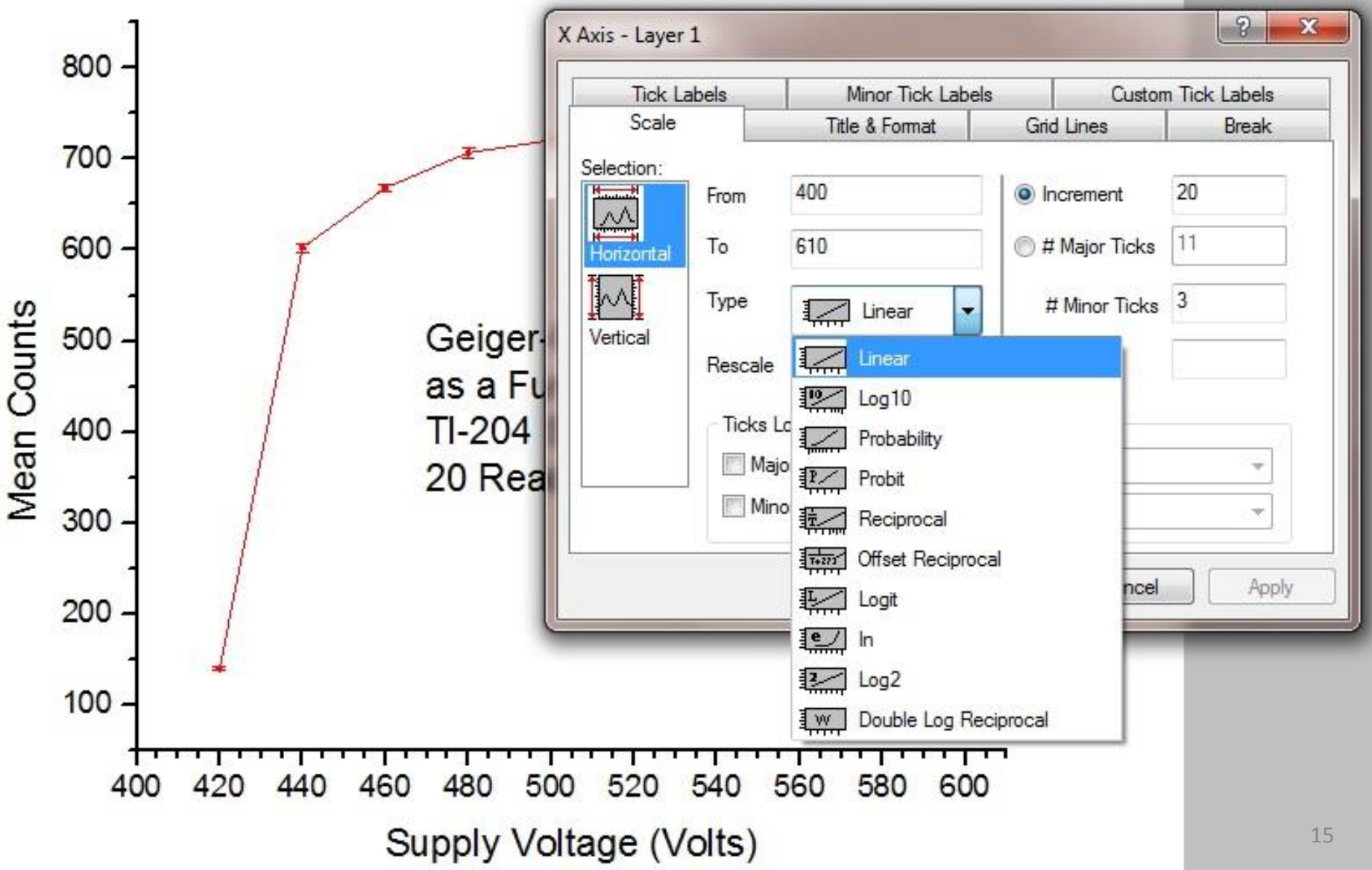
Voilà! A plot!


Mean Counts
800
700
600
500
400
300
200
100
400
420
440
460
480
500
520
540
560
580
600
Supply Voltage (Volts)
Geiger-Muller Tube #3 Response
as a Function of Supply Voltage
Tl-204 Source 33 mm from Detector
20 Reads at 5 sec. 0.5 V Threshold

Changing Plotting Parameters

- Double click on axes to change parameters therein
- Click on “T” on the left bar to add text (like the title of your graph!)
- If you entered text for “Long name” and “Units” in the headers of the “Sheet” in the “Book” they will appear as axis labels.

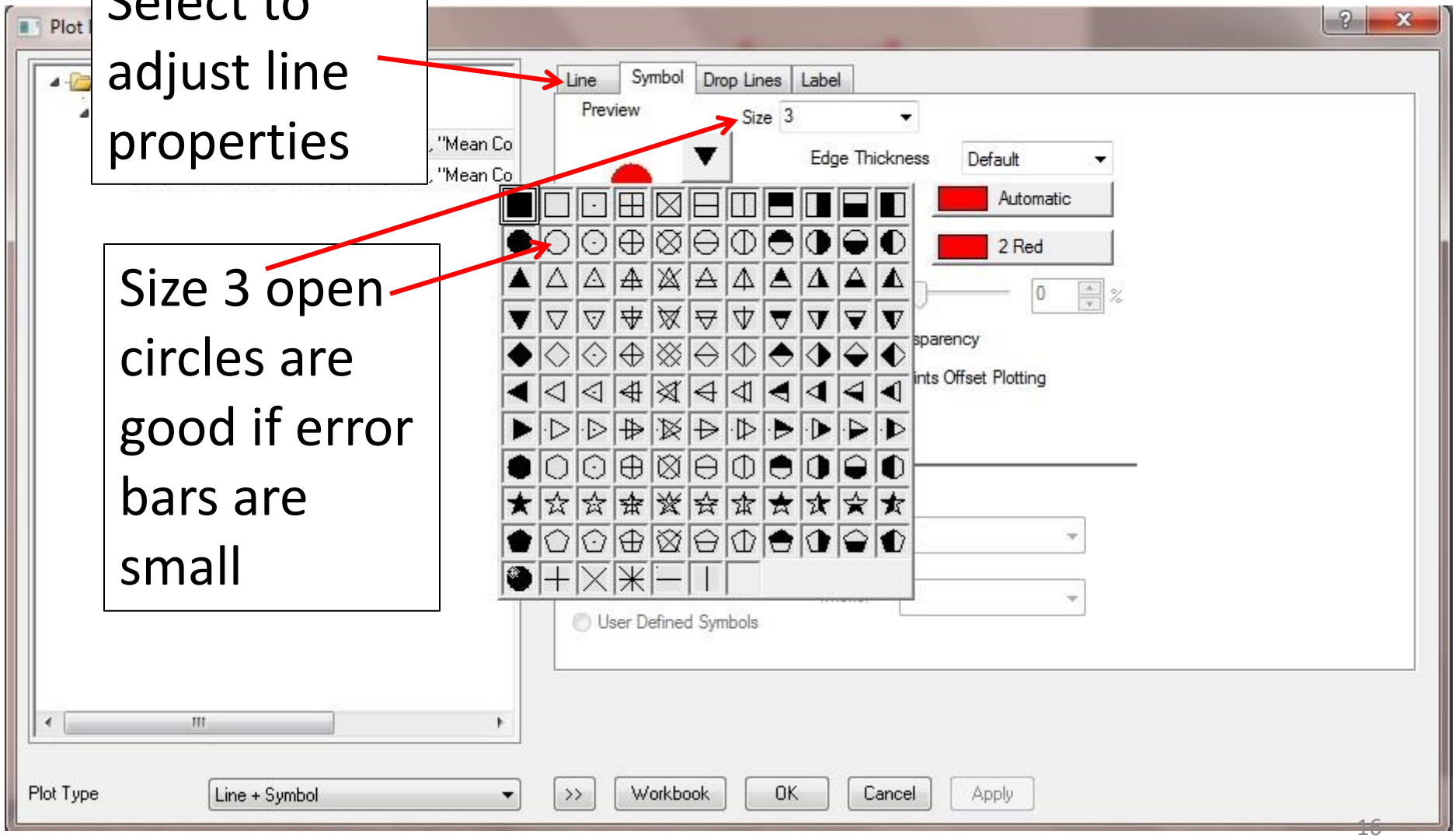
Adjust Axis Parameters



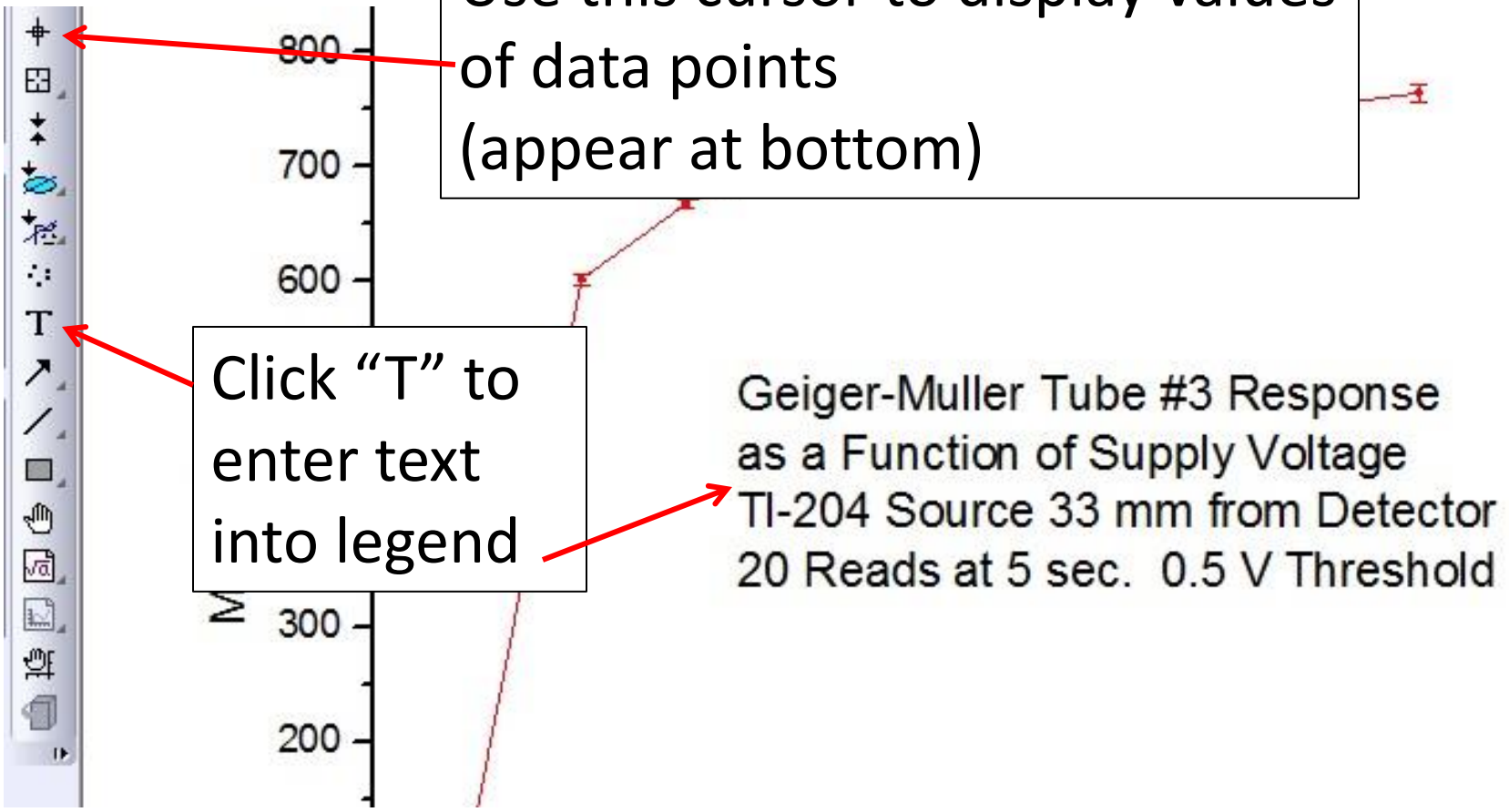
Adjust Plot Details

Select to adjust line properties

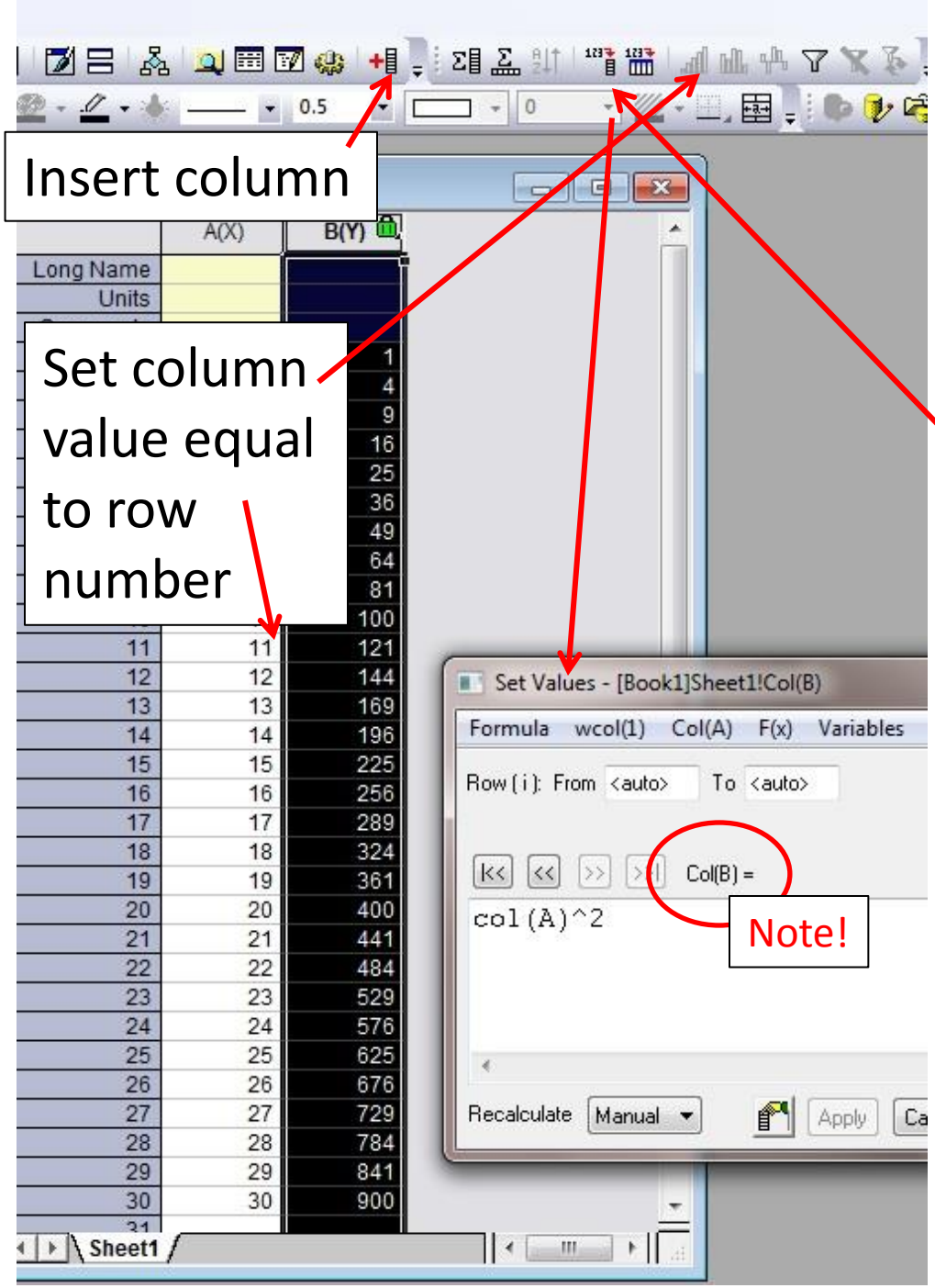
Size 3 open circles are good if error bars are small



Adding a Legend



Column Manipulations



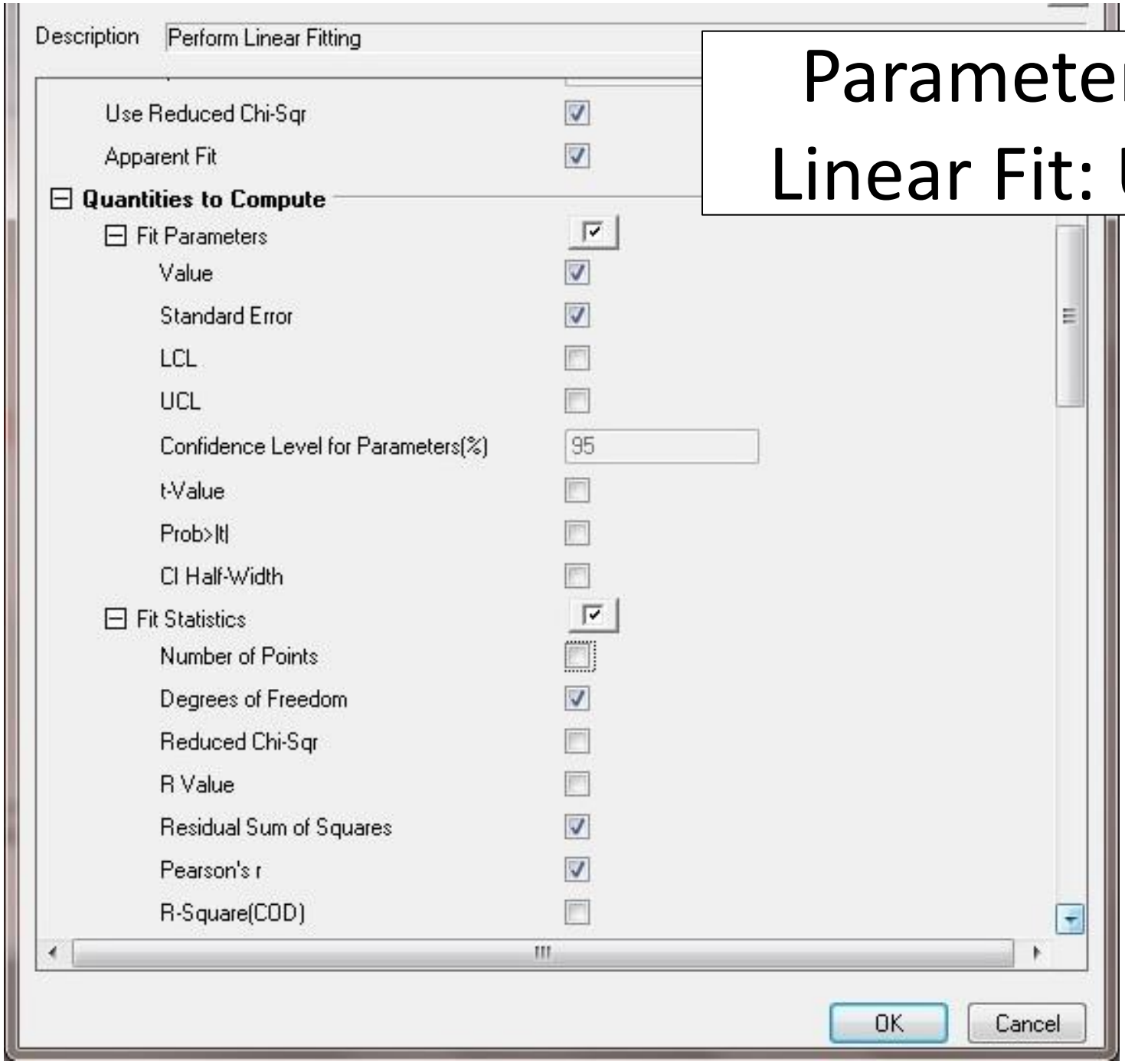
Select column where results are to appear, here B.
Click the icon to “Set column values”
Syntax: You are telling the program to generate in the new column rows whose values are the result of operating on the adjacent values in the named column [in this case col(A)] in the specified manner [in this case squared]

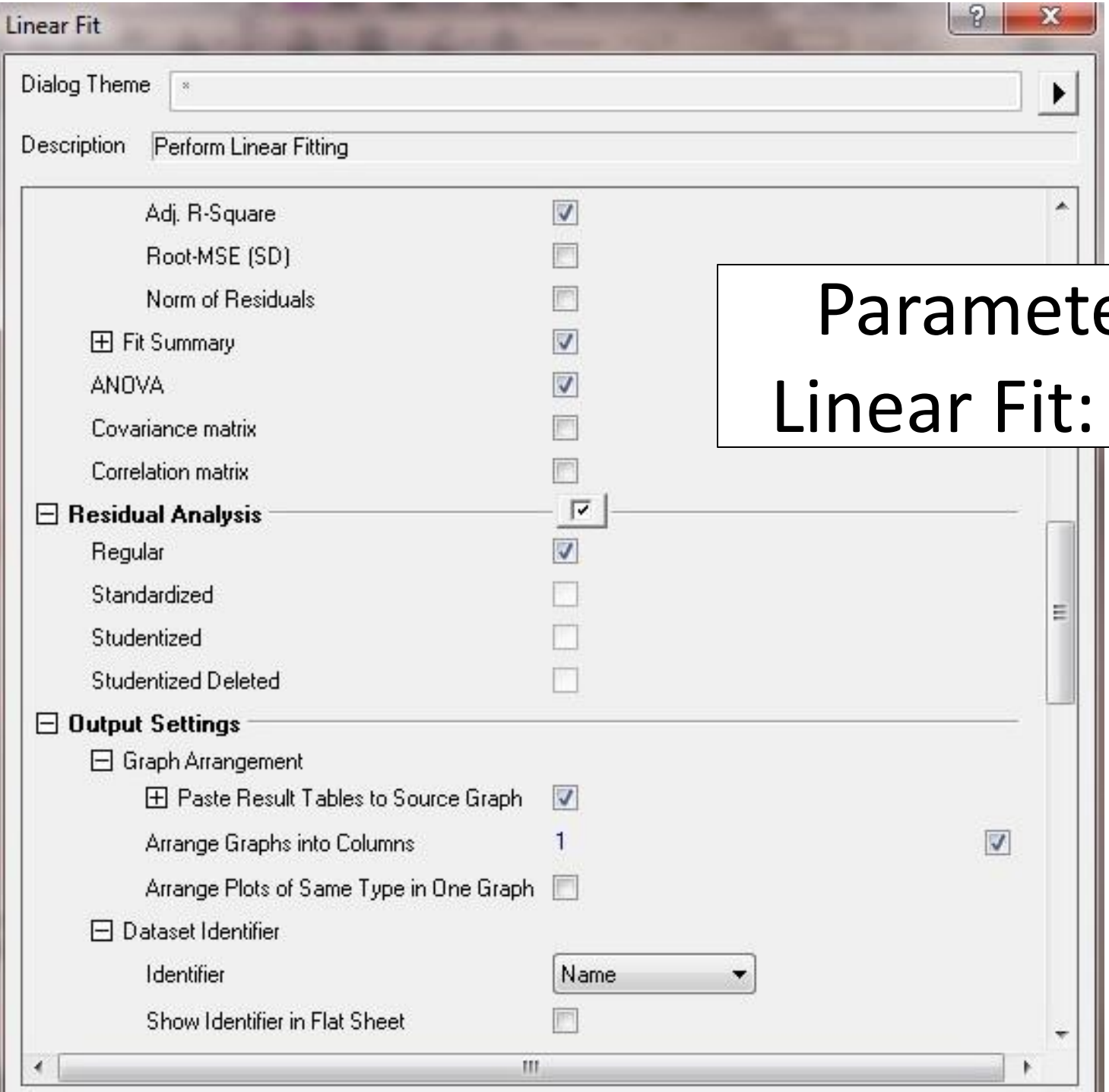
Linear Least Squares Fitting

- Plot data!
- Analysis: Fitting: Linear Fit: Open Dialog
  - “Residual sum of squares” is another name for chi squared
  - Check “R-value” or “R-square” (this is the correlation coefficient)
  - Assure that it is checked!
  - Also check “Reduced chi Sqr” (for G-M experiment)
  - Also assure that Residual Analysis: Regular is checked
  - Uncheck the “Adj. R-Square” and “Pearson’s r” (their formulas are not the typical ones for the correlation coefficient R or r)

- Alternatively
  - Enter all data into Excel
  - Calculate mean, Standard Deviation and Standard Deviation of the Mean
  - Transfer relevant rows to empty Book in Origin
  - Worksheet/Transpose/Dialog/OK
- Plot:Line:scatter
- Select columns to plot
  - A(X) for X
  - B(Y) for Y
  - C2(Y) for YEr
- Adjust symbols, line, axes and labels as appropriate
- Use “T” icon on left to generate plot label

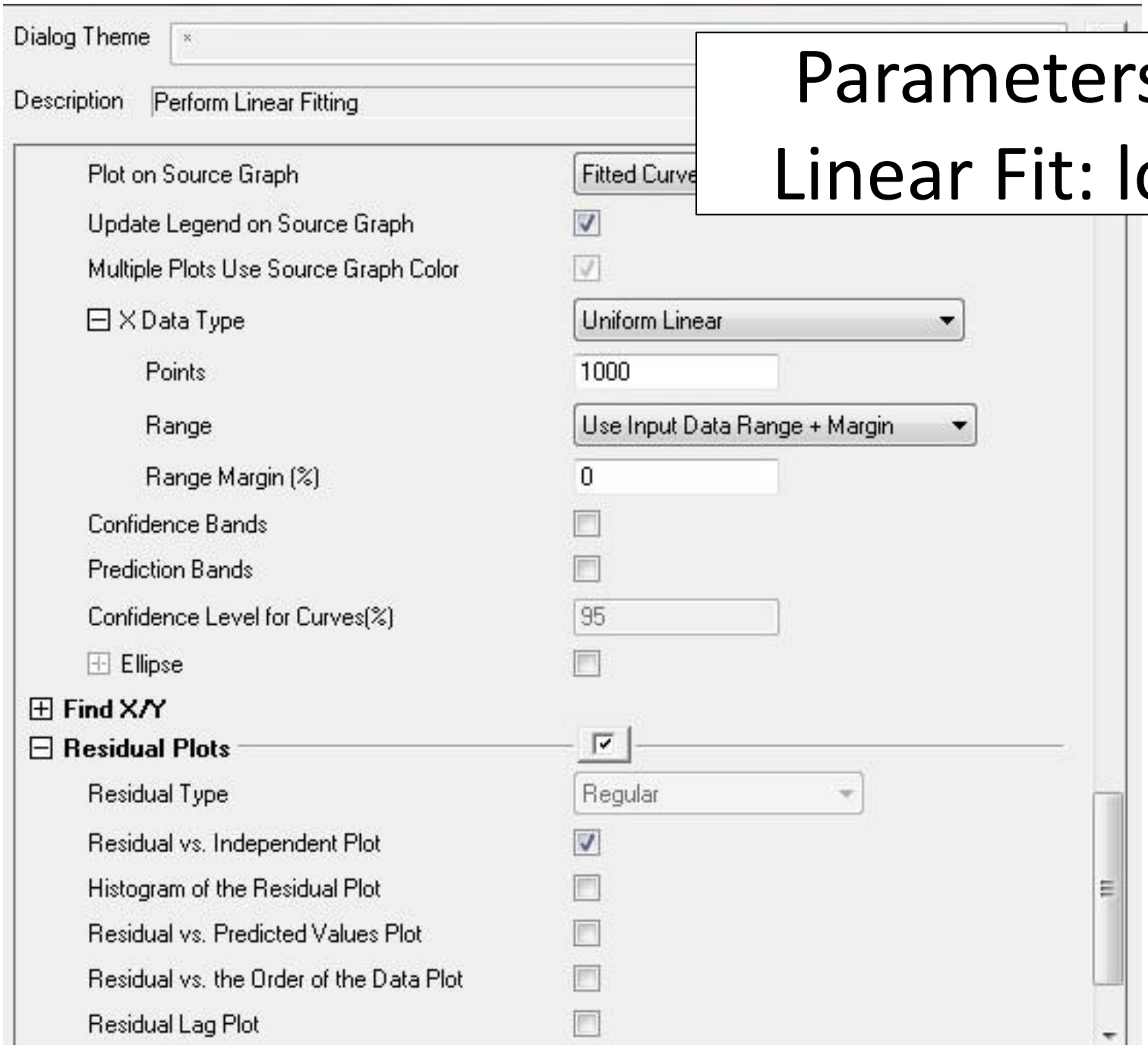
Parameters for Linear Fit: Upper





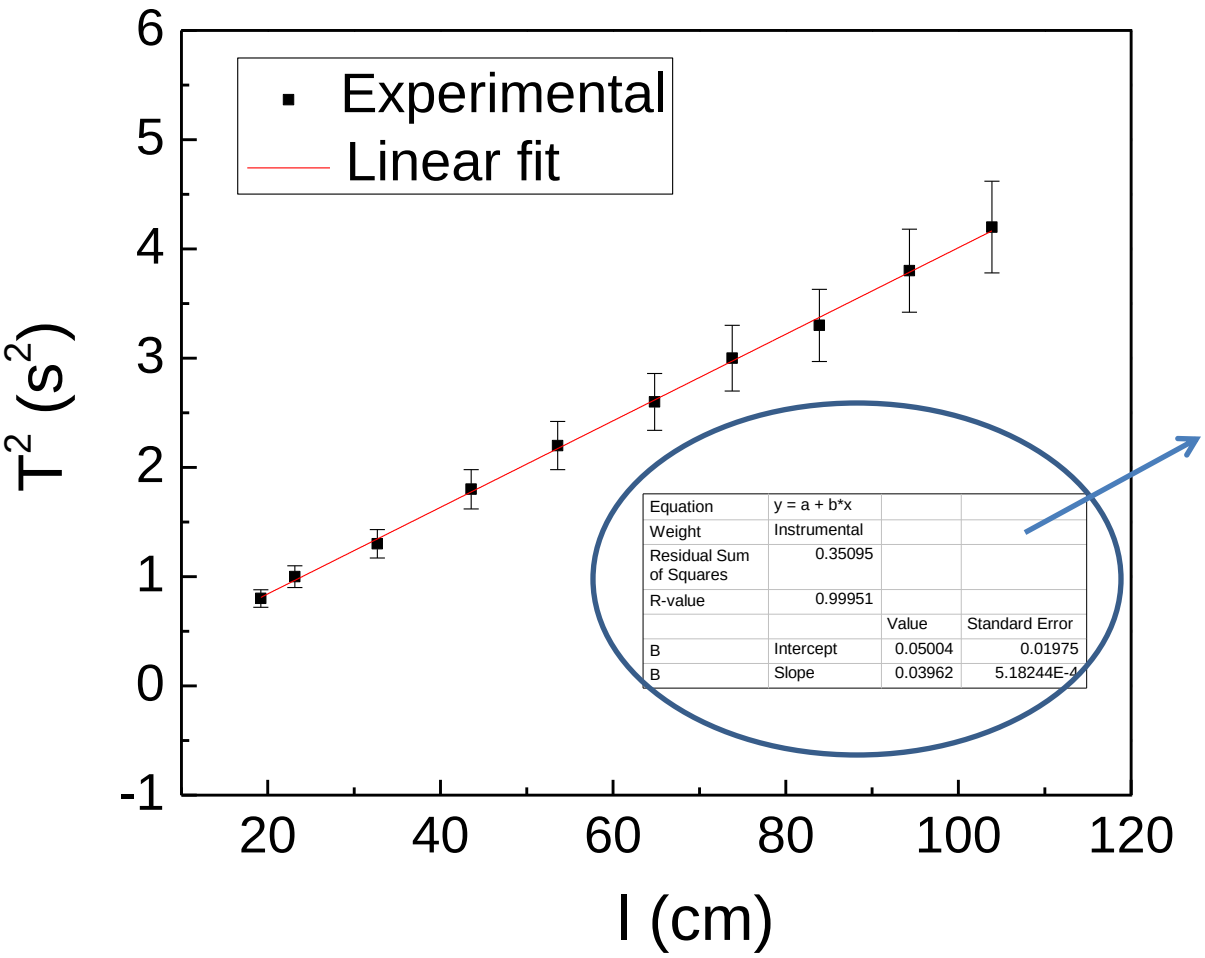
Parameters for Linear Fit: Middle

Parameters for Linear Fit: lower



Plotted Data with Fit and Error Bars

Example: pendulum experiment



Info about the linear fit (next slide)

- Info about the linear fit (from previous slide graph):

Equation	y = A + Bx			
Weight	Instrumental			Considering error bars
Residual Sum of Squares	0.35095			Chi-squared ($\chi 2$) considering error bars
R-value	0.99951			Correlation coefficient (r or R)
		Value	Standard Error	Value and Absolute error
A	Intercept	0.05004	0.01975	
B	Slope	0.03962	5.18244E-4	

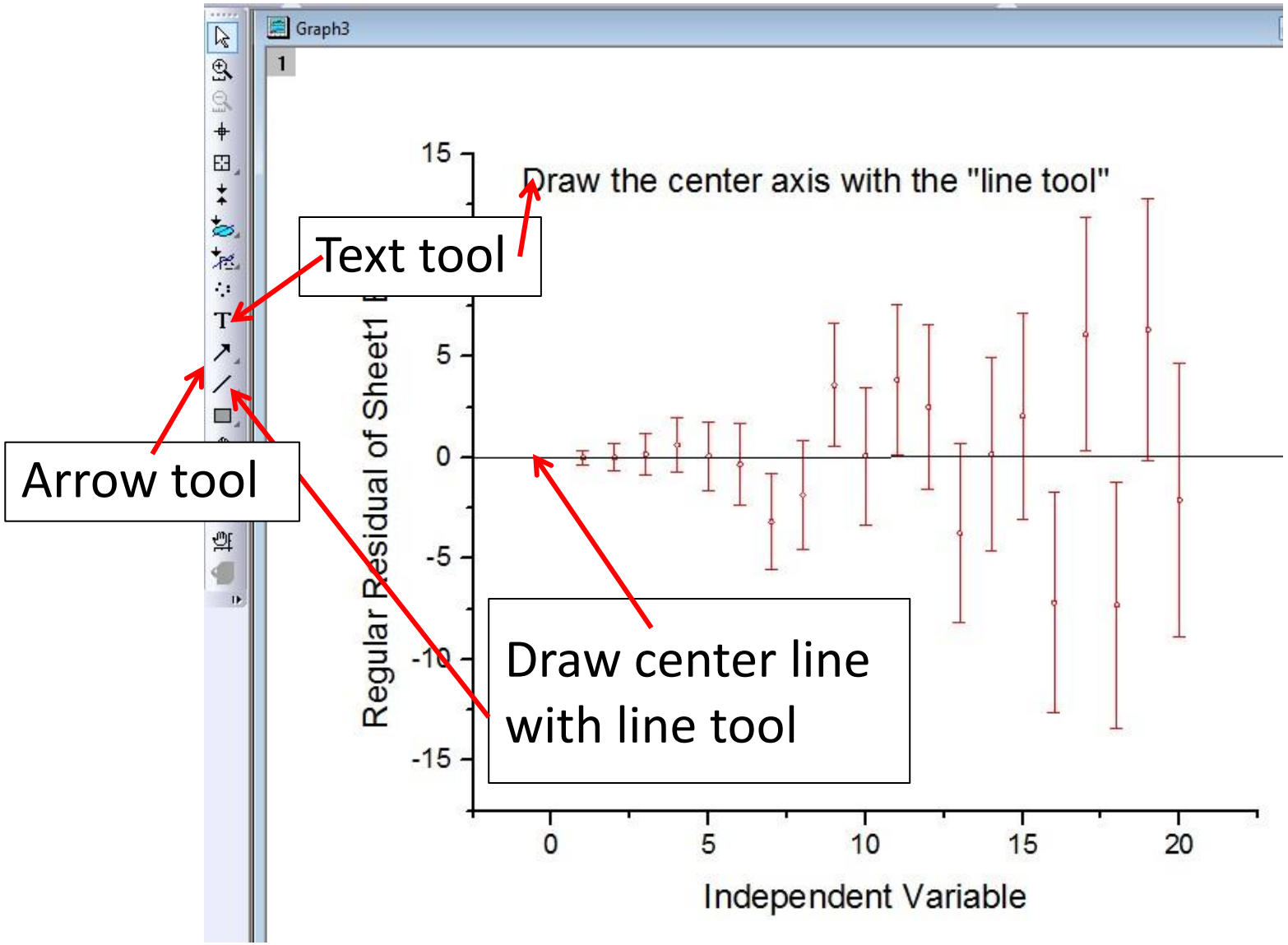
Residual Plot with Error Bars

- Residual values will appear as a new column in the sheet “FitLinearCurve1”
- Retrieve error bar magnitudes from original calculations [column SEM(yEr)]
- Plot residual values with error bars as a function of y-data as usual

A3(X2)	A4(Y2)	A(Y2)
Independent Variable	Regular Residual of Sheet1 C"Y"	Error bars
1	0.01774	0.34
2	-0.30879	0.68
3	0.55795	1.02
4	0.52993	1.36
5	-0.27298	1.7
6	1.20008	
7	-3.66752	
8	0.78302	
9	2.06146	
10	3.06399	
11	-5.2316	
12	0.91976	
13	-4.87794	
14	-7.84186	
15	5.47137	5.1
16	0.73543	5.44
17	0.65829	5.78
18	4.92268	6.12
19	5.60616	6.46
20	-2.40591	6.8

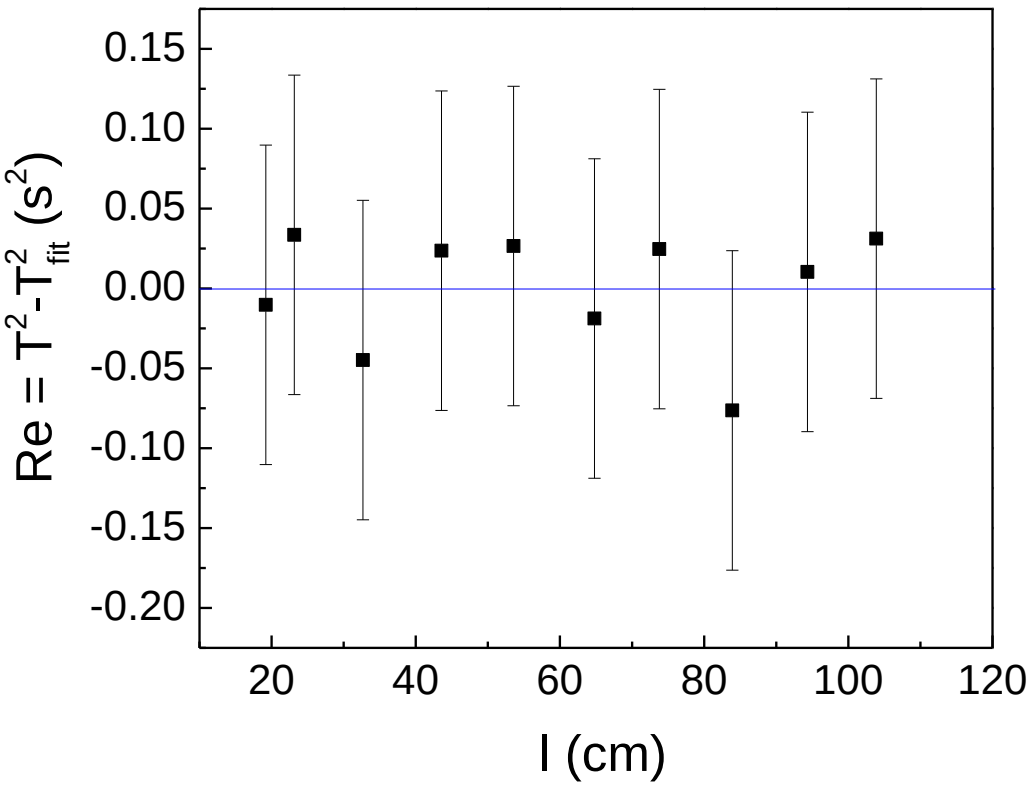
Data for Residual Plot: FitLinearCurve1 Sheet

Test Fit Residuals with Error Bars



Residual plot for the example on slide 24 (pendulum experiment)

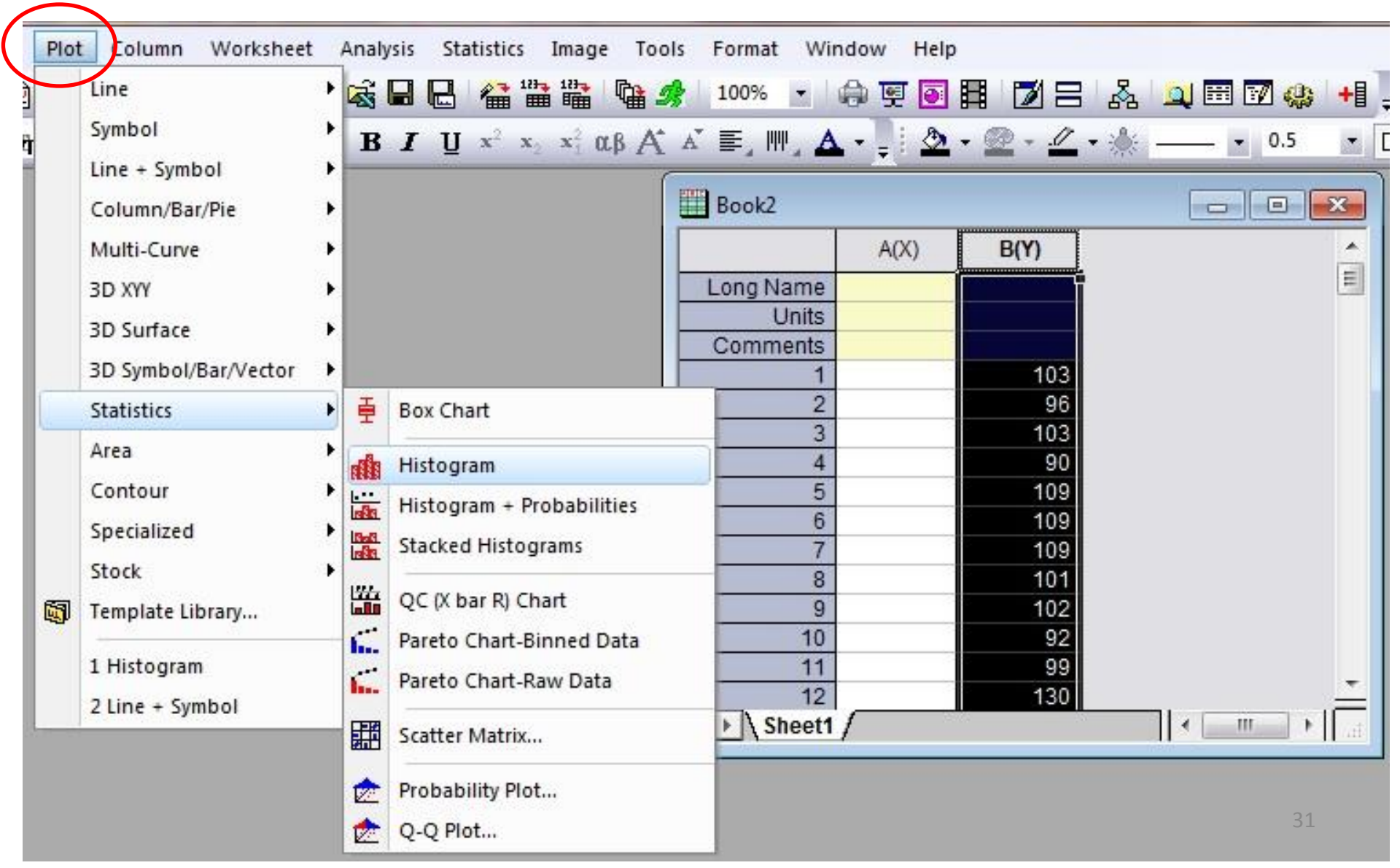
Plotting $Re = T^2 - T^2_{fit}$ vs. l with error bars for δT^2:



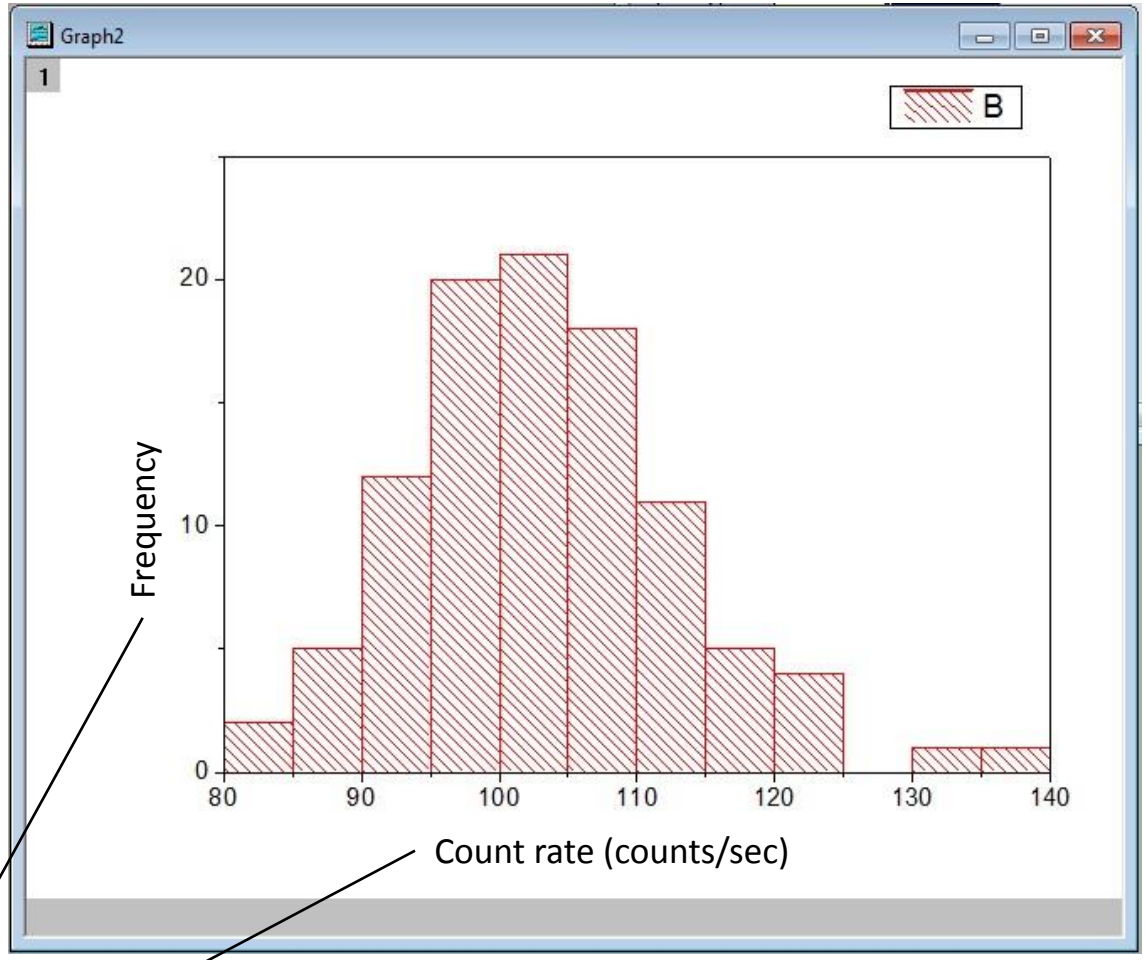
Generating and Fitting a Histogram

- Import data to be plotted into a Y-column of a new book/worksheet.
  - The x-column doesn't work, even if you have only one set of data to generate a histogram. Don't ask.
- Block those data (CTRL click above column)

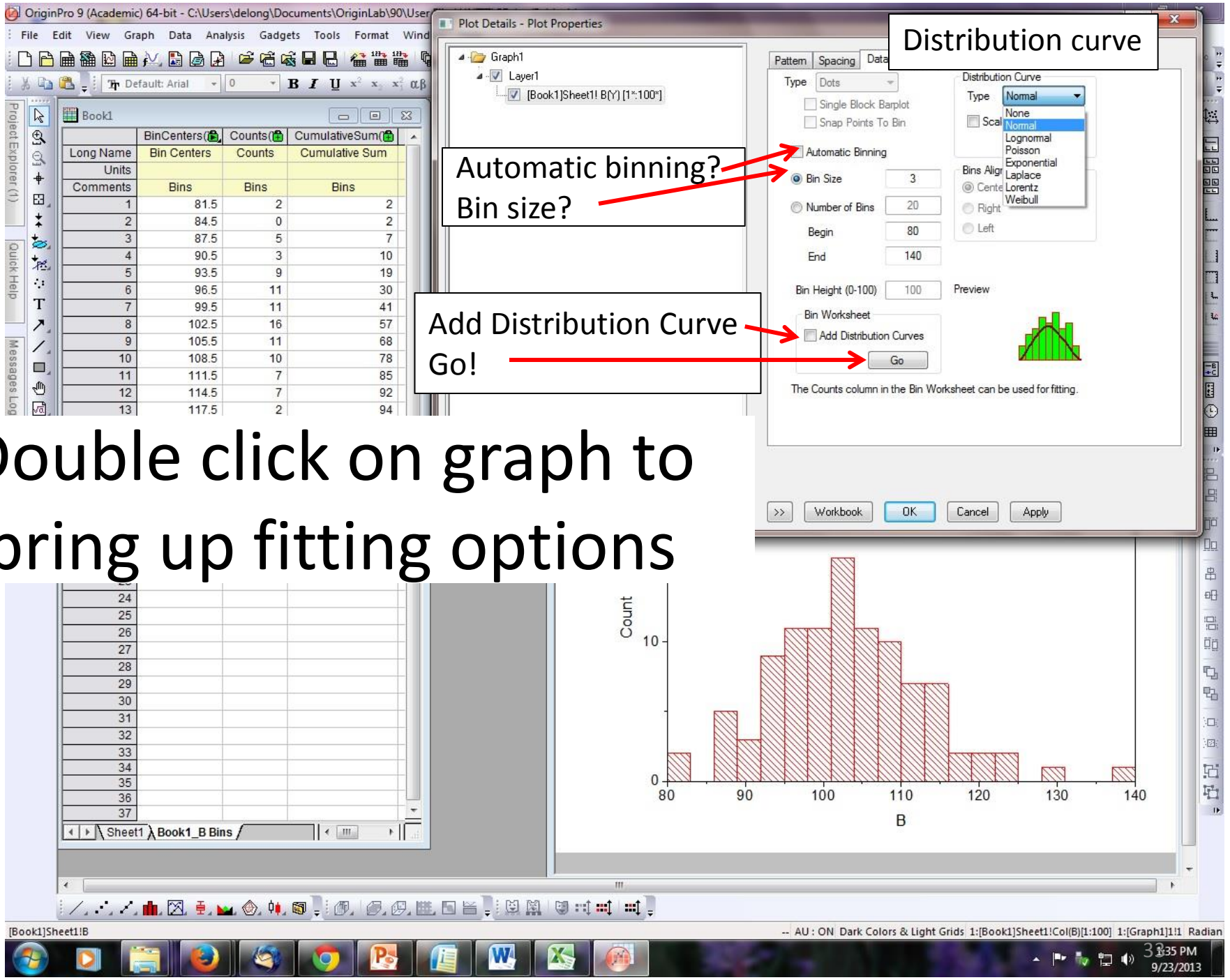
To Plot a Histogram



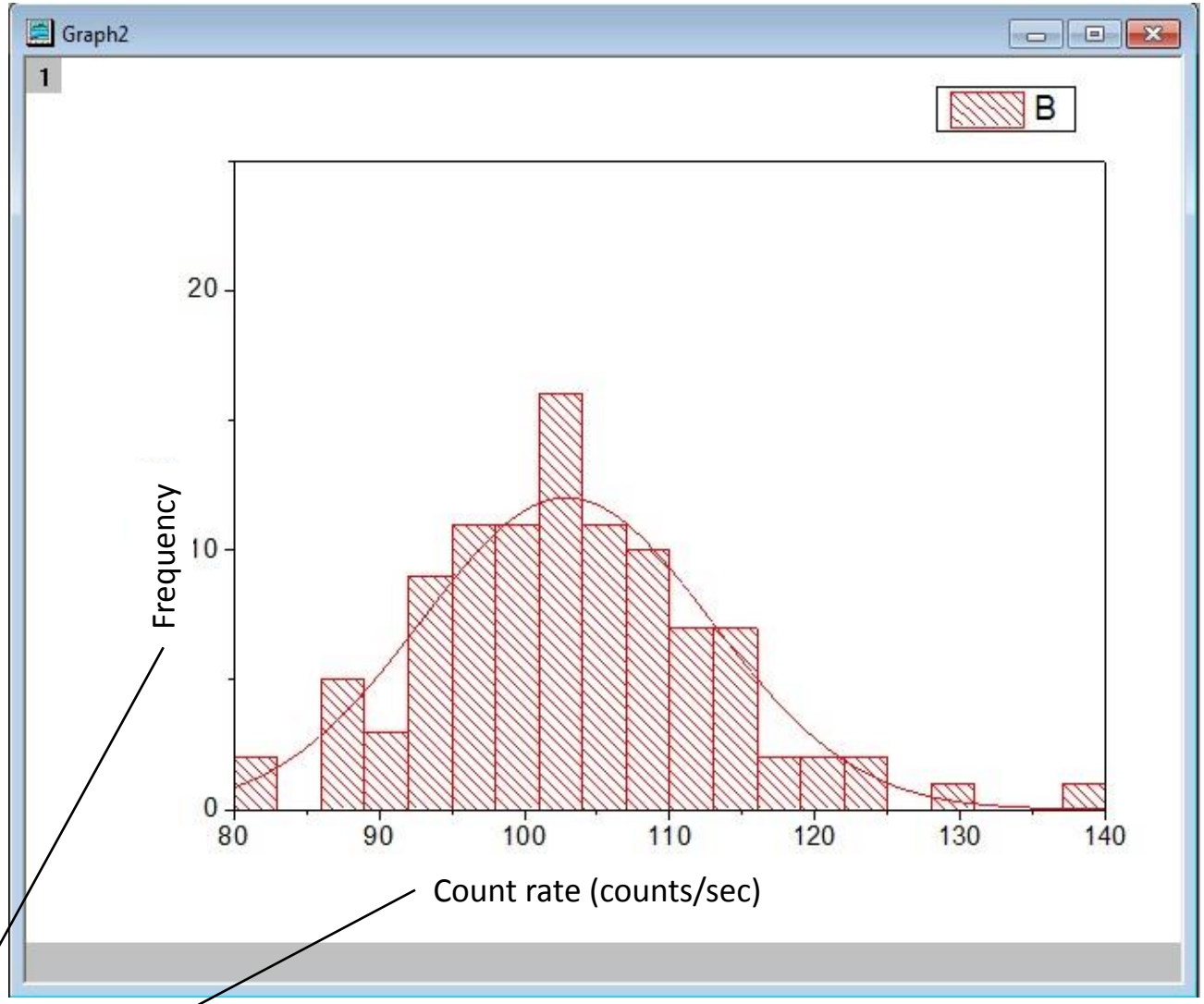
Initial Histogram



Example of axis labels for the Geiger-Müller experiment

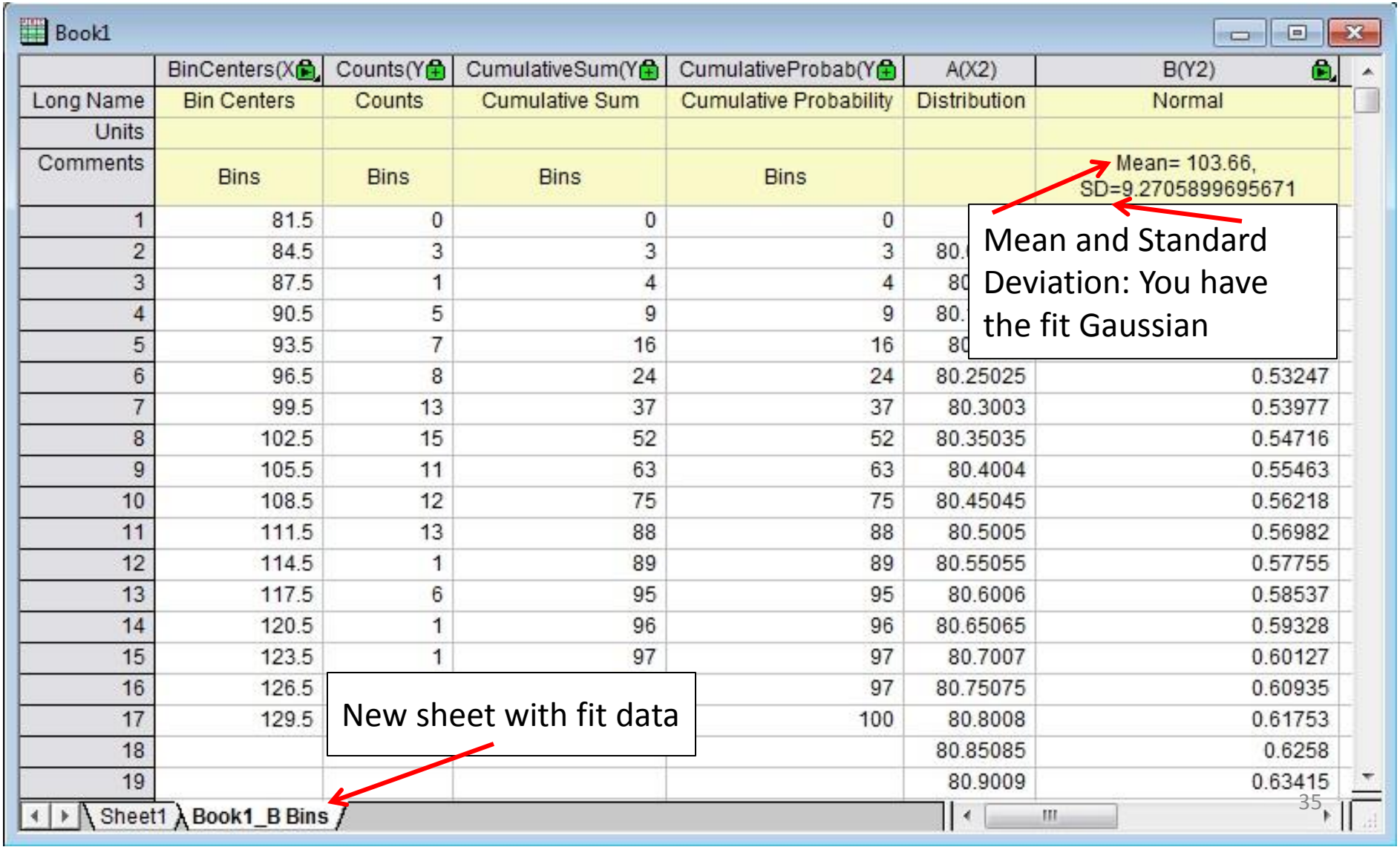

Distribution curve
Automatic binning?
Bin size?
Add Distribution Curve
Go!
Double click on graph to bring up fitting options
Plot Details - Plot Properties
Graph1
Layer1
[Book1]Sheet1! B(Y) [1*:100*]
Pattern
Spacing
Type
Dots
Single Block Barplot
Snap Points To Bin
Automatic Binning
Bin Size
3
Number of Bins
20
Begin
80
End
140
Bin Height (0-100)
100
Preview
Bin Worksheet
Add Distribution Curves
Go
The Counts column in the Bin Worksheet can be used for fitting.
Distribution Curve
Type
Normal
None
Normal
Lognormal
Poisson
Exponential
Laplace
Lorentz
Weibull
Workbook
OK
Cancel
Apply
Book1
BinCenters
Counts
CumulativeSum
Long Name
Bin Centers
Counts
Cumulative Sum
Units
Comments
Bins
Sheet1
Book1_B Bins
Count
B
[Book1]Sheet1!B
AU : ON
Dark Colors & Light Grids
1:[Book1]Sheet1!Col(B)[1:100]
1:[Graph1]1!1
Radian
9/23/2013

Histogram with Gaussian Overlay



Example of axis labels for the Geiger-Müller experiment

Histogram Fit Sheet

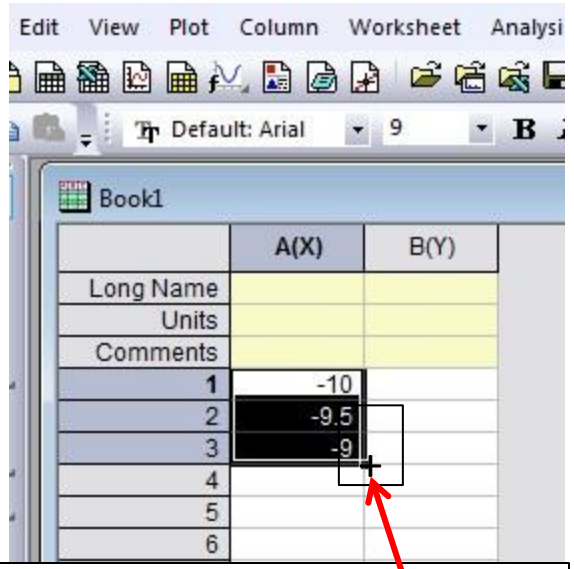


Generating a Function

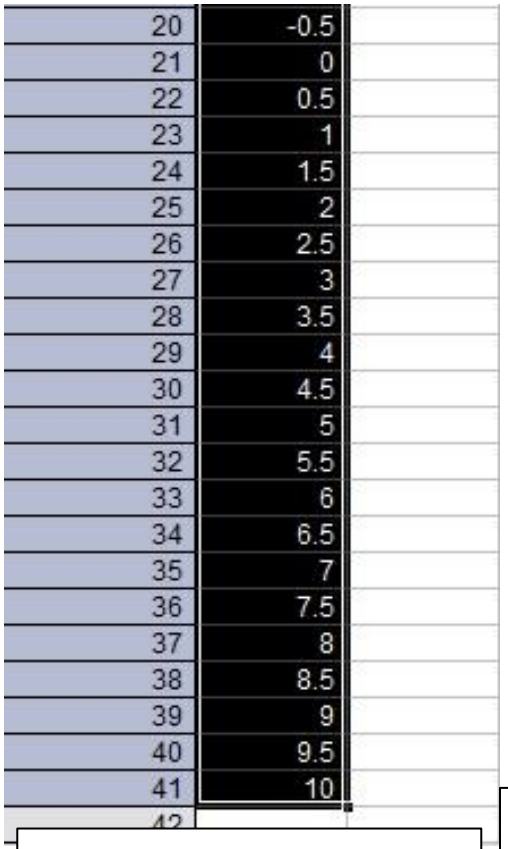
Sometimes you want to plot a function over some interval

- Enter the first few values of the independent variable (next slide)
- Block those values
- Set the cursor at the bottom right of the column until the cursor becomes a plus sign (next slide)
- Drag the cursor down for the number of rows corresponding to the range of x that you want to plot
  - To increase the number of rows, click on the bottom cell and hit Enter
- Block column to be used for dependent values
- Set column values: enter expression for function to be plotted
- Plot!
- Adjust axes, titles and legend to suit taste.

Example: $Y = X^3$ for -10<X<10

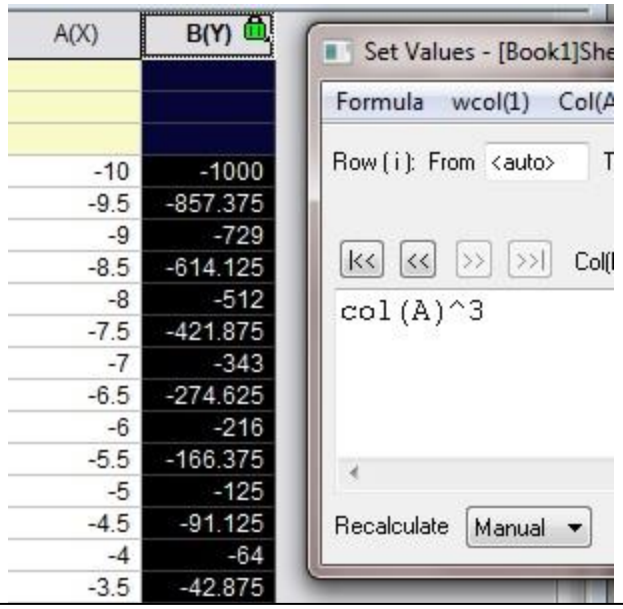


Enter 2-3 values and block
Move cursor to bottom right corner of cell (+)



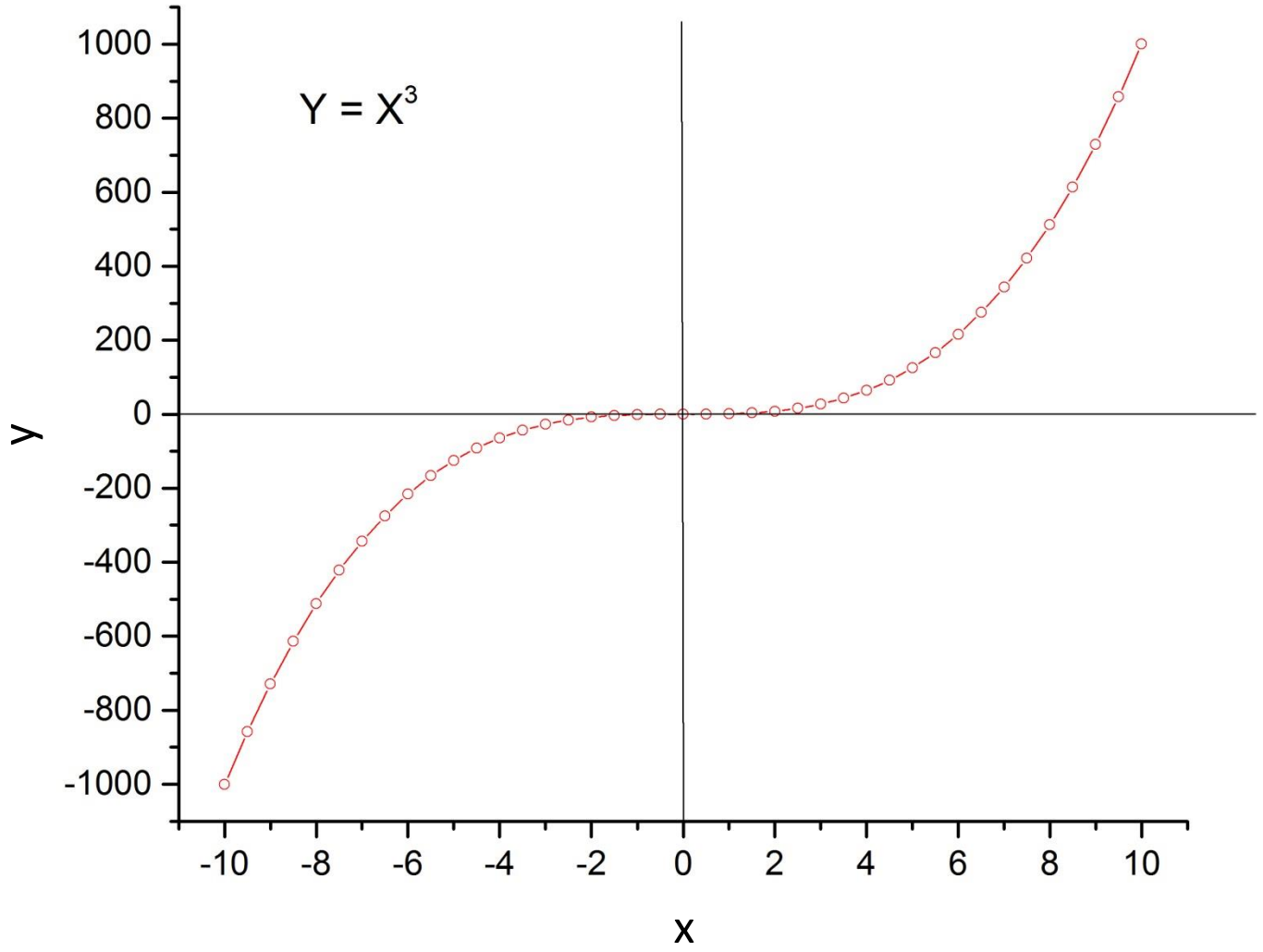
Drag cursor to last x-value

Set values



Enter the cube of the value in col(A) in the blocked column

Voilà!

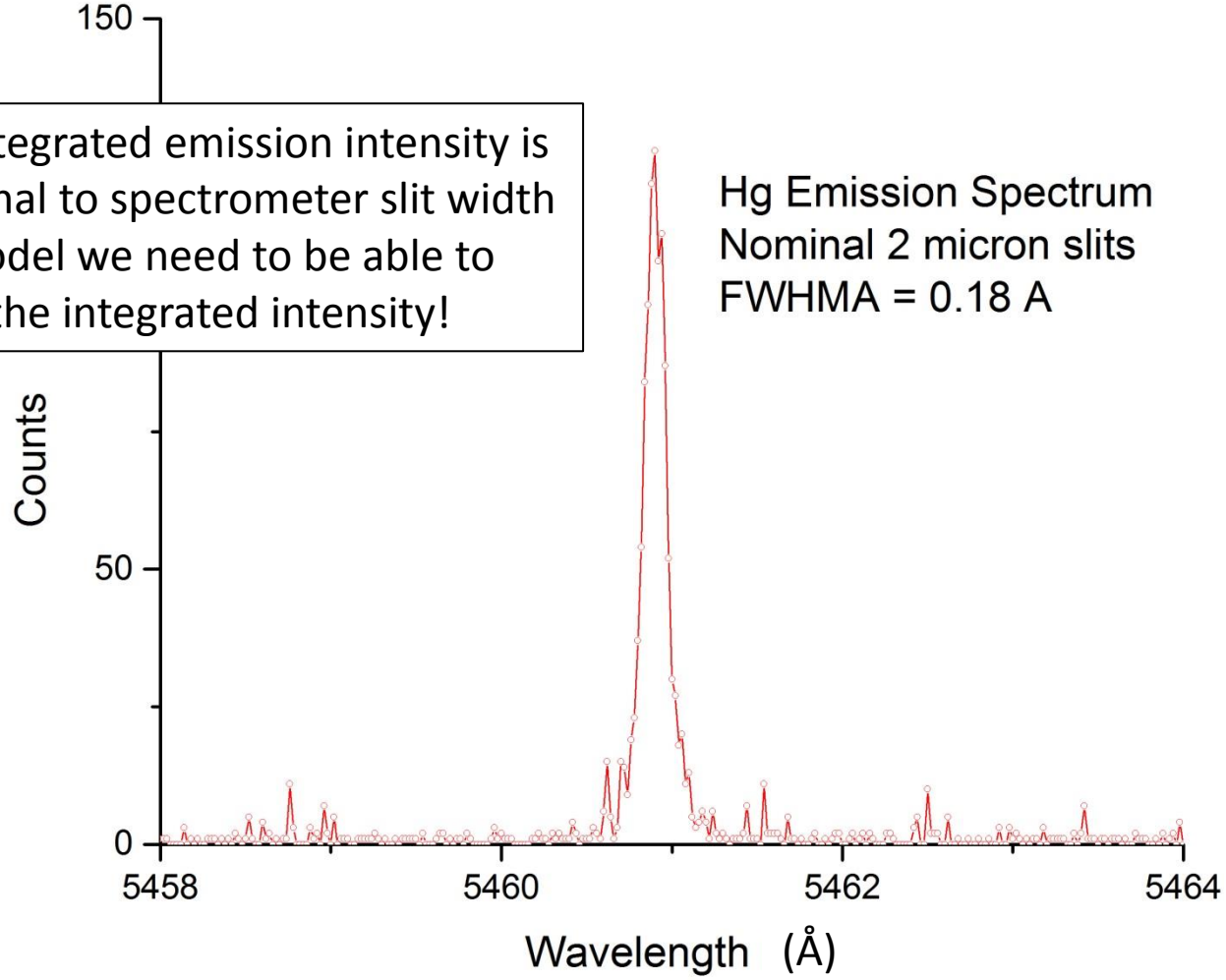

Y = X3
1000
800
600
400
200
0
-200
-400
-600
-800
-1000
y
-10
-8
-6
-4
-2
0
2
4
6
8
10
x

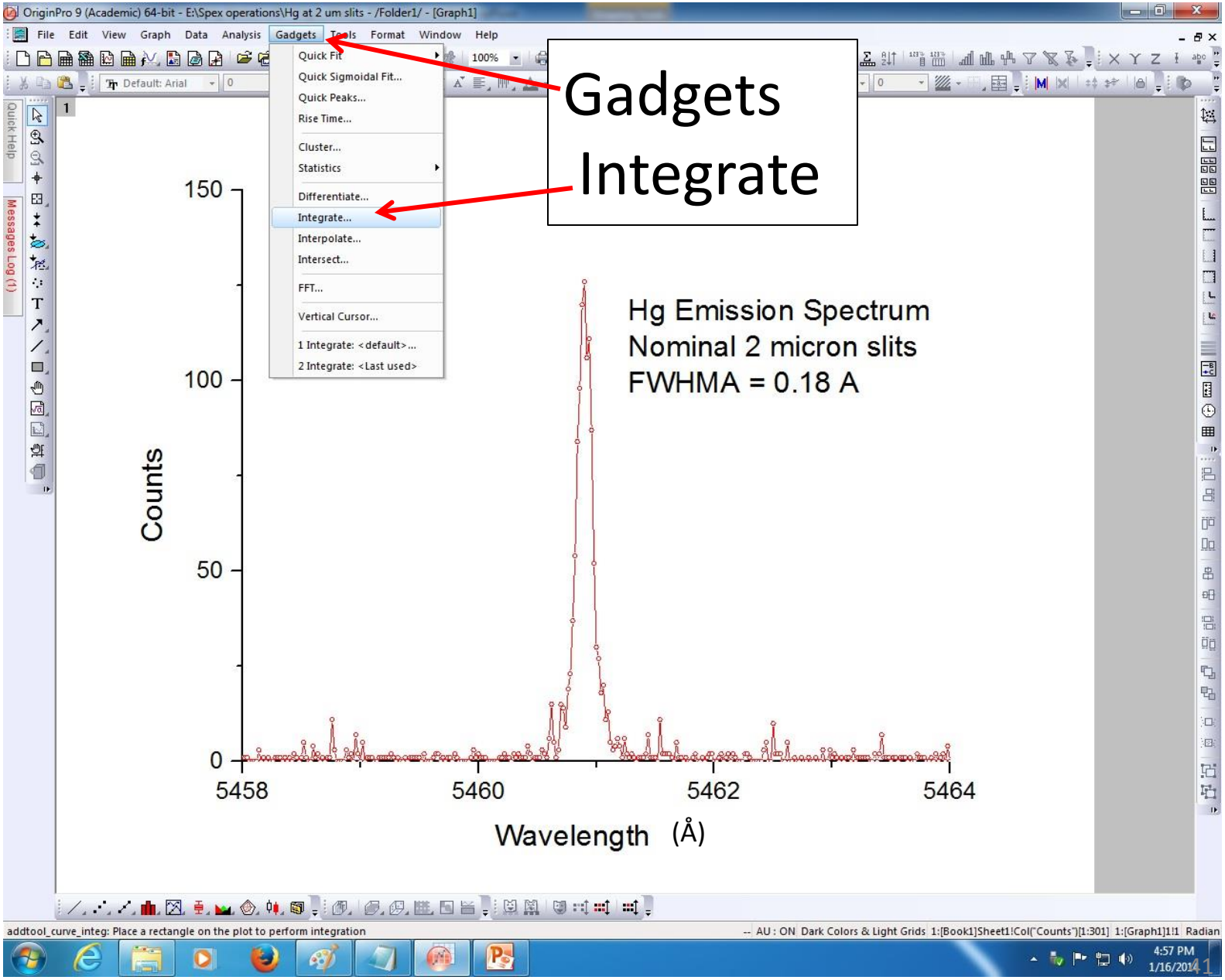
Integrating with Origin

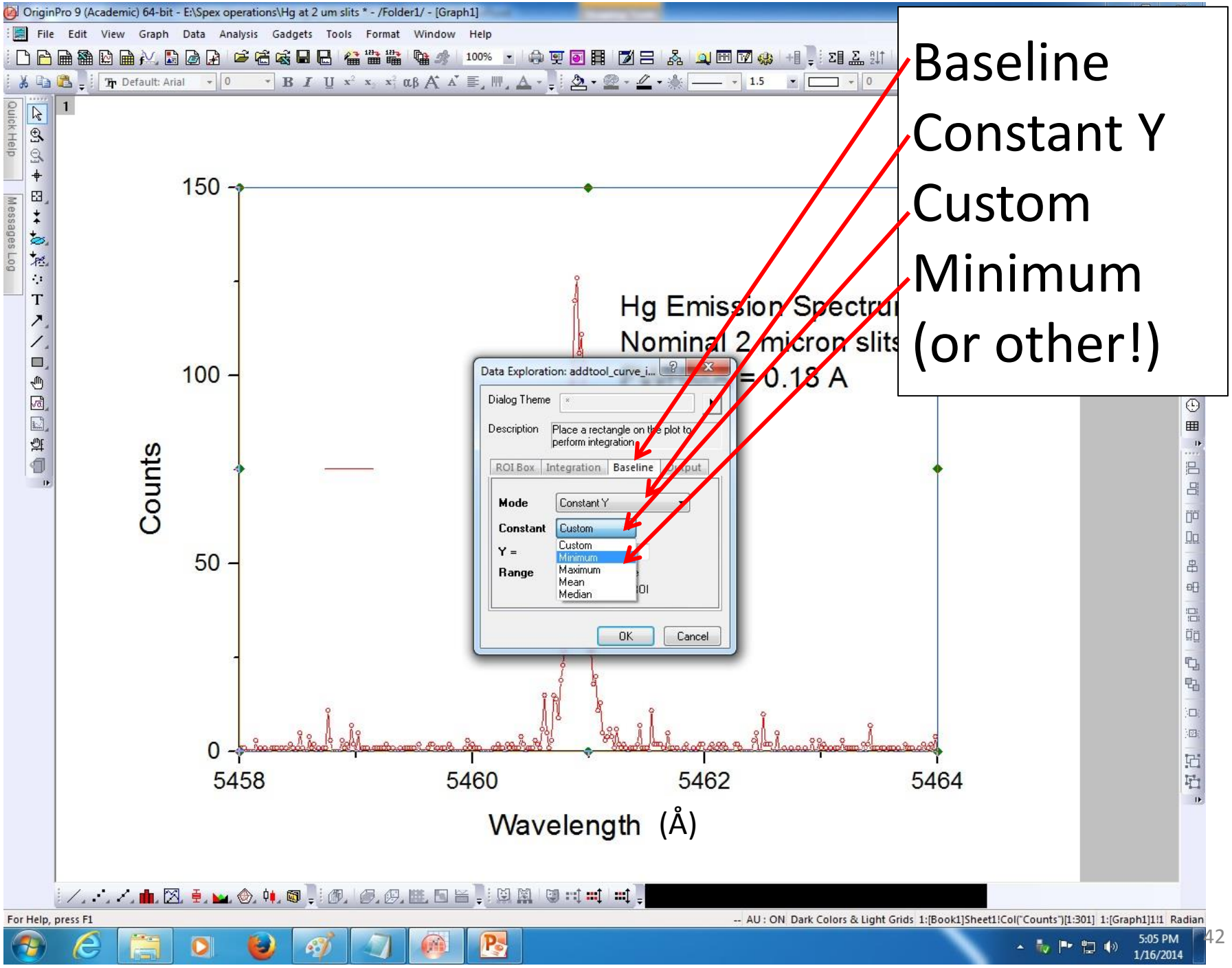
- Useful analyzing optical data
  - Integrated intensity of an emission peak
- Chemical analysis: finding the total amount of material from an absorption curve
  - Beer's Law
  - Concentration is proportional to absorbance
- Easier and more accurate than olden times when Professor Lüty plotted data an paper, cut out curve with scissors and weighed paper!

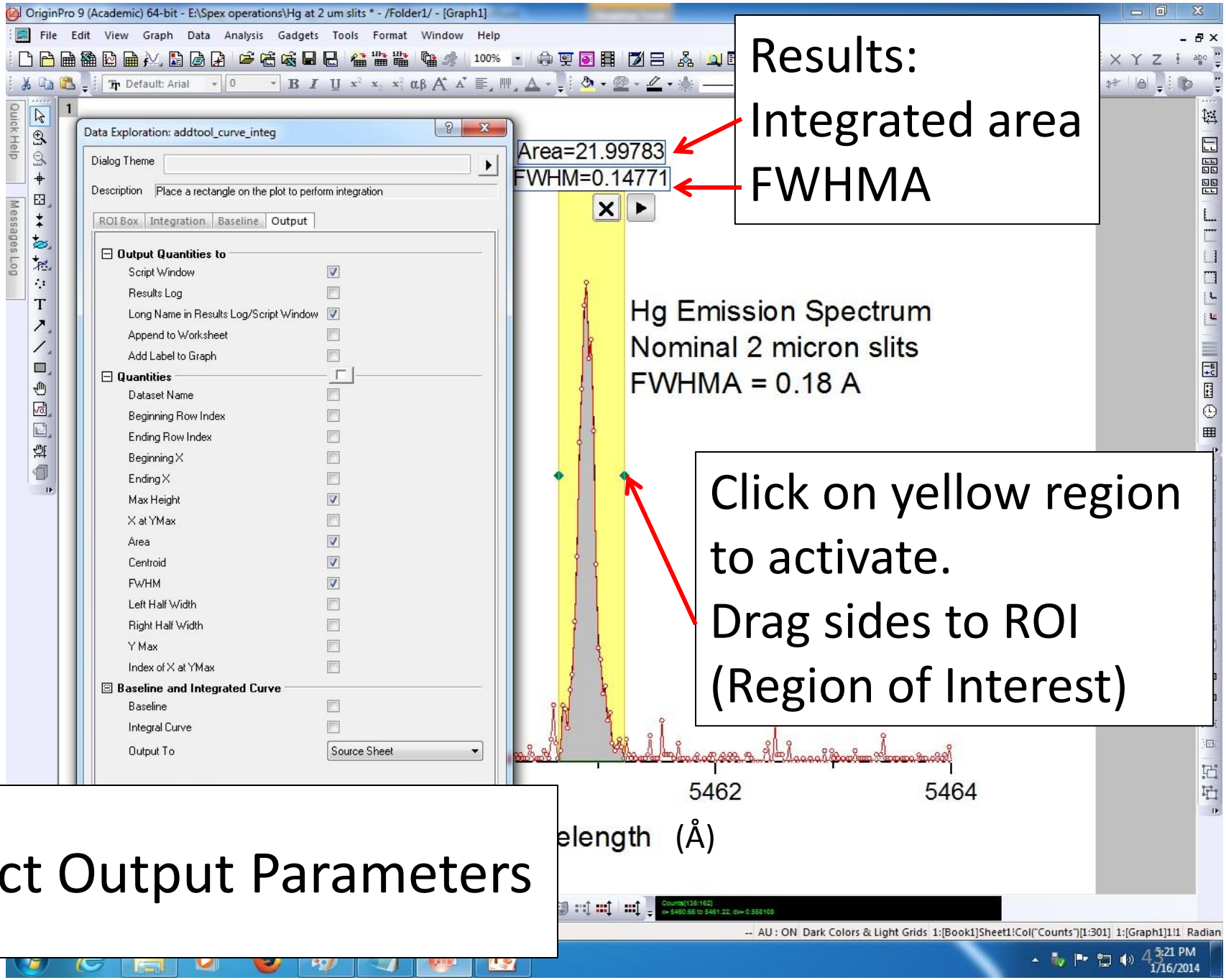
Mercury Emission Spectrum

Model: Integrated emission intensity is proportional to spectrometer slit width
To test model we need to be able to calculate the integrated intensity!




Gadgets
Integrate
Hg Emission Spectrum
Nominal 2 micron slits
FWHMA = 0.18 A
Counts
Wavelength (Å)
150
100
50
0
5458
5460
5462
5464
File Edit View Graph Data Analysis Gadgets Tools Format Window Help
Quick Fit
Quick Sigmoidal Fit...
Quick Peaks...
Rise Time...
Cluster...
Statistics
Differentiate...
Integrate...
Interpolate...
Intersect...
FFT...
Vertical Cursor...
1 Integrate: <default>...
2 Integrate: <Last used>
addtool_curve_integ: Place a rectangle on the plot to perform integration


Baseline
Constant Y
Custom
Minimum
(or other!)
OriginPro 9 (Academic) 64-bit - E:\Spex operations\Hg at 2 um slits * - /Folder1/ - [Graph1]
File Edit View Graph Data Analysis Gadgets Tools Format Window Help
Hg Emission Spectru
Nominal 2 micron slits
= 0.18 A
Counts
Wavelength (Å)
150
100
50
0
5458
5460
5462
5464
Data Exploration: addtool_curve_i...
Dialog Theme
Description
Place a rectangle on the plot to perform integration
ROI Box
Integration
Baseline
Mode
Constant Y
Constant
Custom
Y =
Range
Custom
Minimum
Maximum
Mean
Median
OK
Cancel
For Help, press F1
5:05 PM
1/16/2014

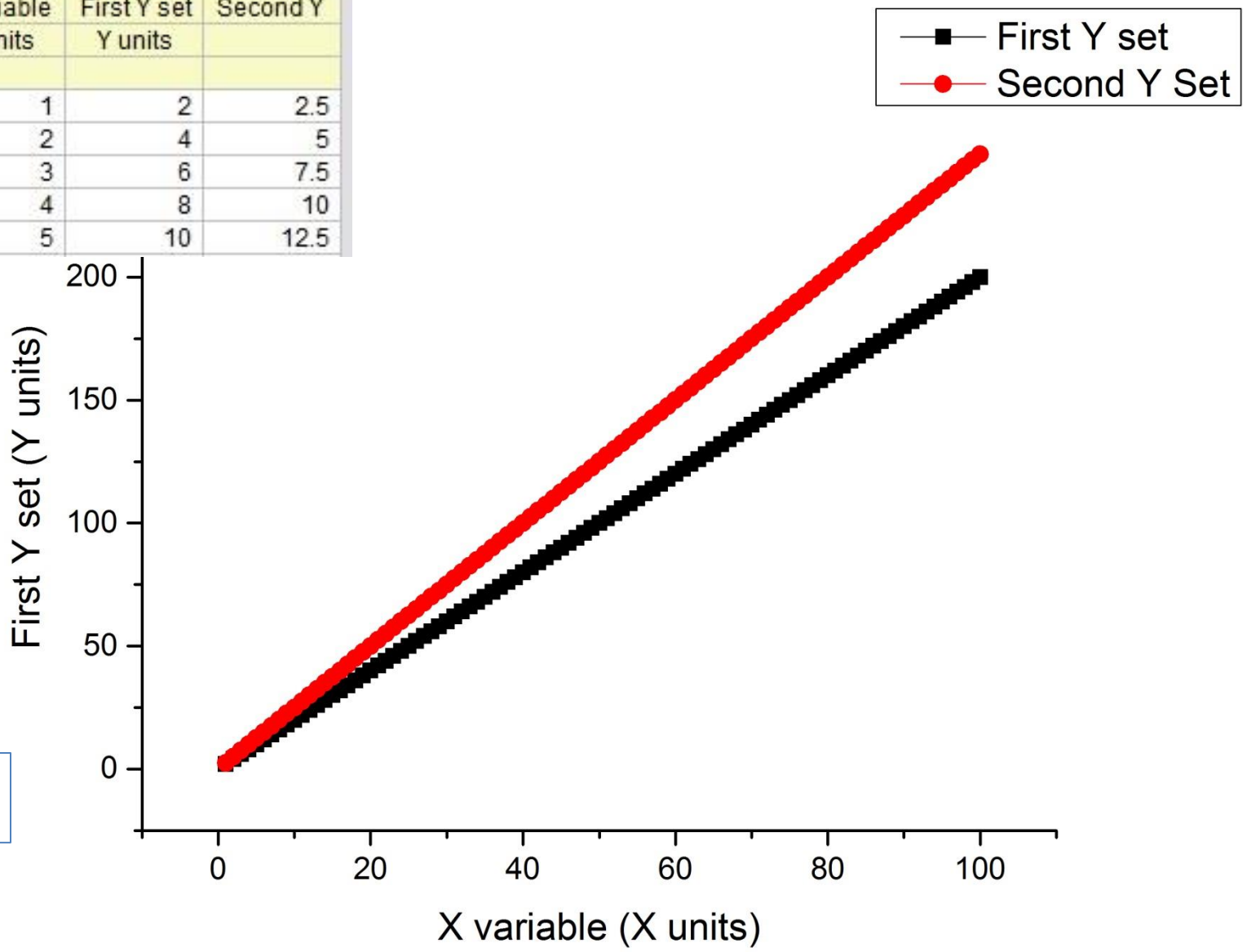

OriginPro 9 (Academic) 64-bit - E:\Spex operations\Hg at 2 um slits * - /Folder1/ - [Graph1]
File Edit View Graph Data Analysis Gadgets Tools Format Window Help
Data Exploration: addtool_curve_integ
Dialog Theme
Description Place a rectangle on the plot to perform integration
ROI Box Integration Baseline Output
Output Quantities to
Script Window
Results Log
Long Name in Results Log/Script Window
Append to Worksheet
Add Label to Graph
Quantities
Dataset Name
Beginning Row Index
Ending Row Index
Beginning X
Ending X
Max Height
X at YMax
Area
Centroid
FWHM
Left Half Width
Right Half Width
Y Max
Index of X at YMax
Baseline and Integrated Curve
Baseline
Integral Curve
Output To
Source Sheet
Area=21.99783
FWHM=0.14771
Hg Emission Spectrum
Nominal 2 micron slits
FWHMA = 0.18 A
5462
5464
elength (Å)
Results:
Integrated area
FWHMA
Click on yellow region
to activate.
Drag sides to ROI
(Region of Interest)
Select Output Parameters

Multiple Plots on a Graph

- Most common: several values of y with a common x
  - Import data
    - Simply block copy and import from Excel
    - File:Import:Multiple ASCII
      - Assumes data are in ASCII format!
      - Requires manipulation of columns after importing
  - You will have multiple columns with one headed by X and the others Y1, Y2…
  - Label each column and give units
  - Block contents of each column to be plotted (click above)
  - Plot: Line and symbol: Line and symbol

Book1

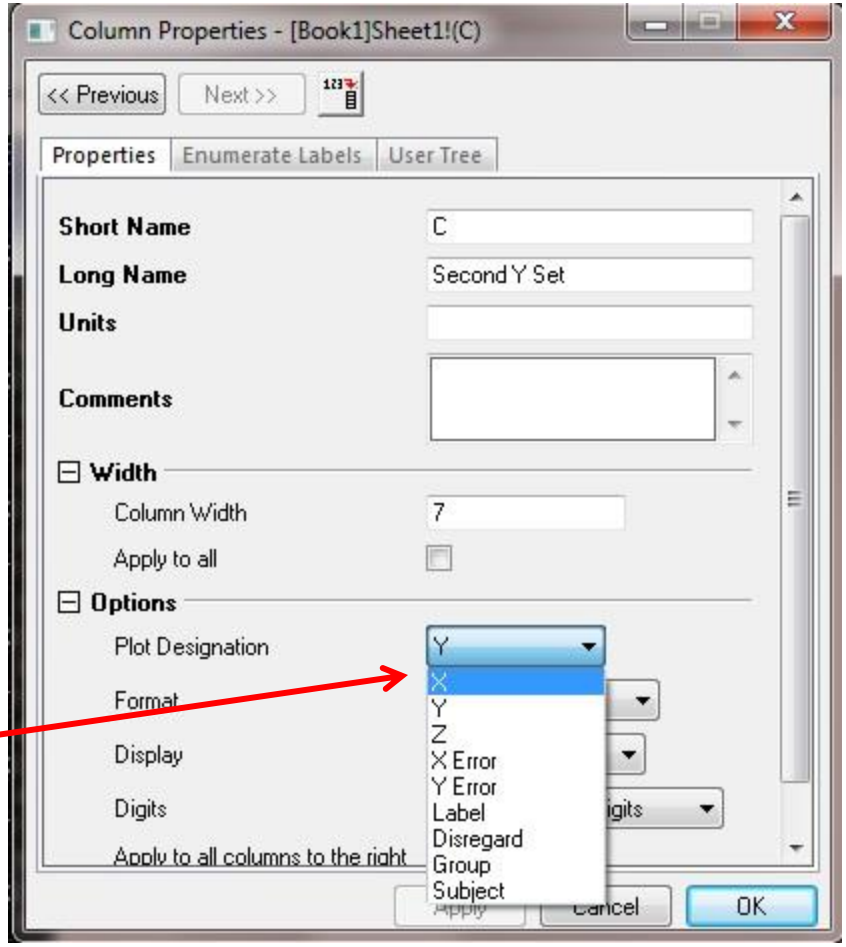
	A(X)	B(Y)	C(Y)
Long Name	X variable	First Y set	Second Y
Units	X units	Y units	
Comments			
1	1	2	2.5
2	2	4	5
3	3	6	7.5
4	4	8	10
5	5	10	12.5



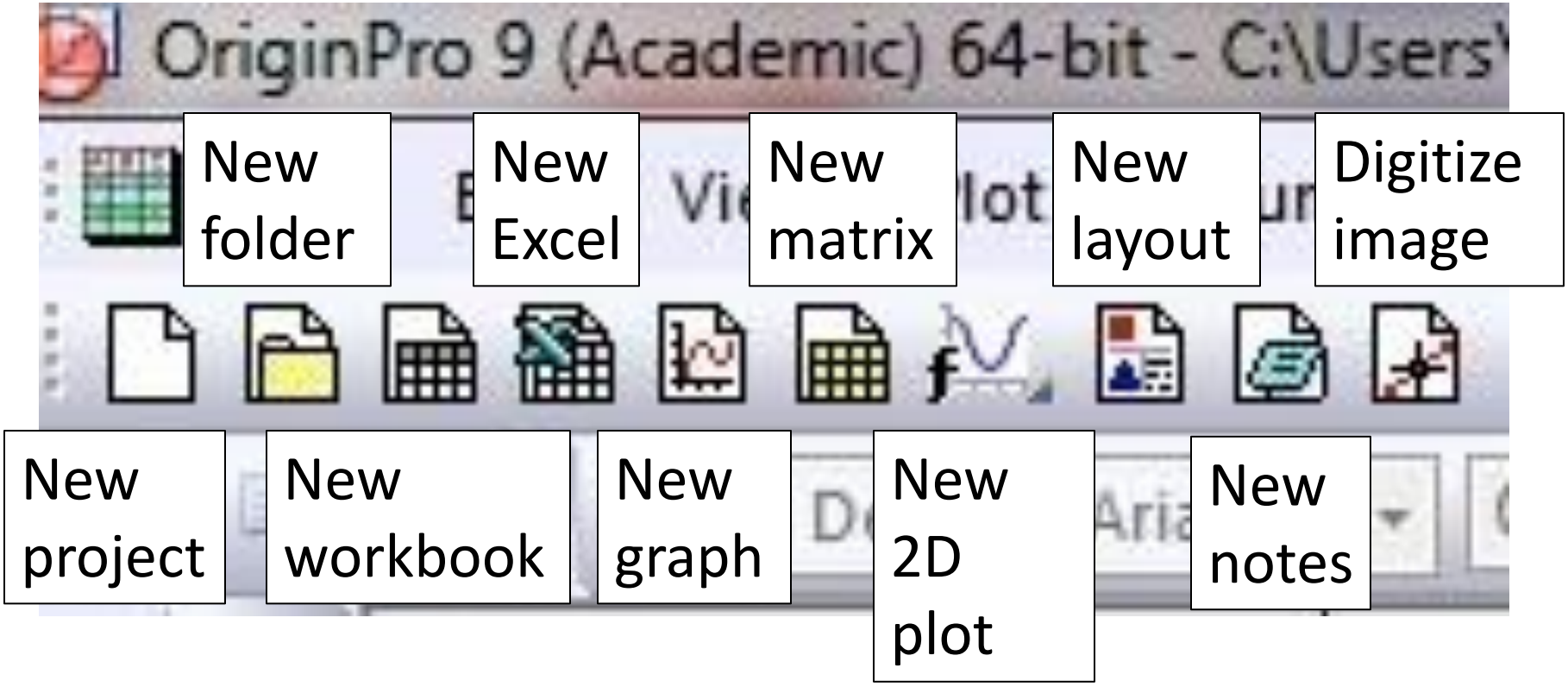
Voilà!

Multiple Plots, Continued

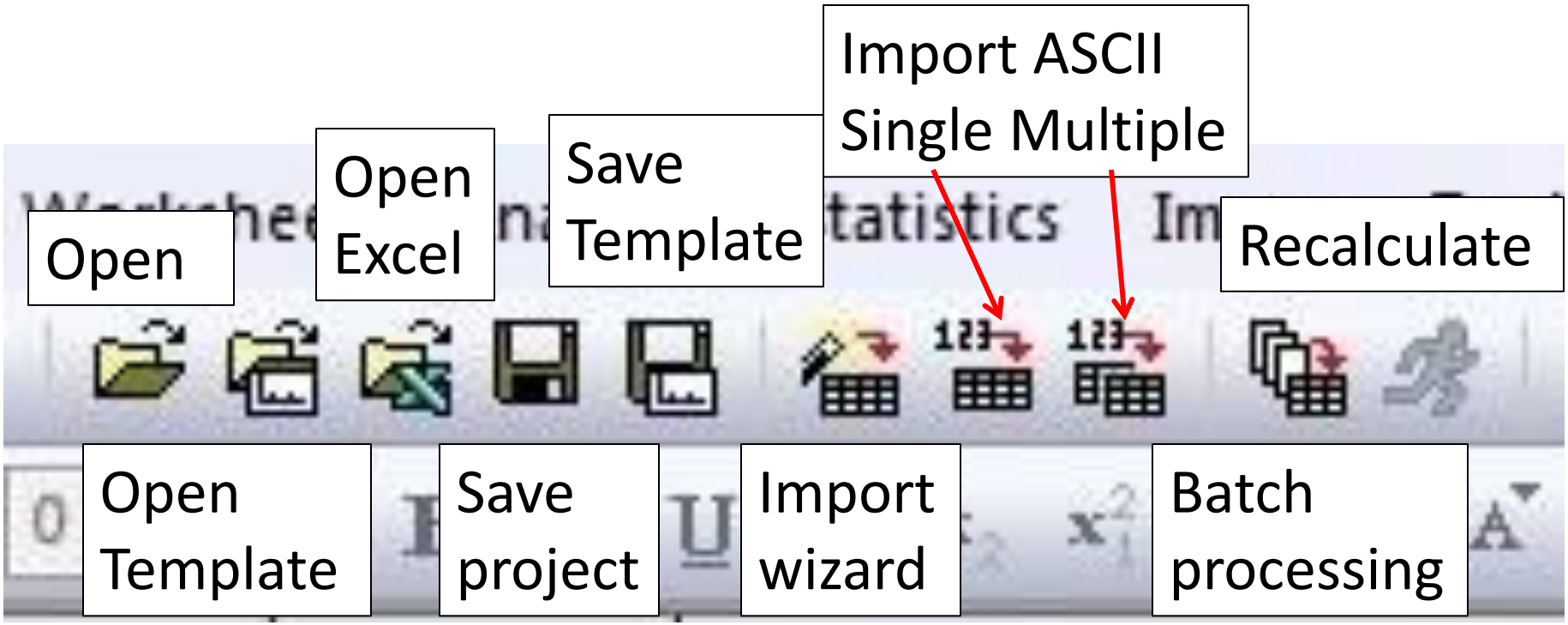
- If multiple plots have different x values
  - Obviously now you have at least four columns of data
  - Double click on the header cell of your second set of x-values
  - Designate second column as x



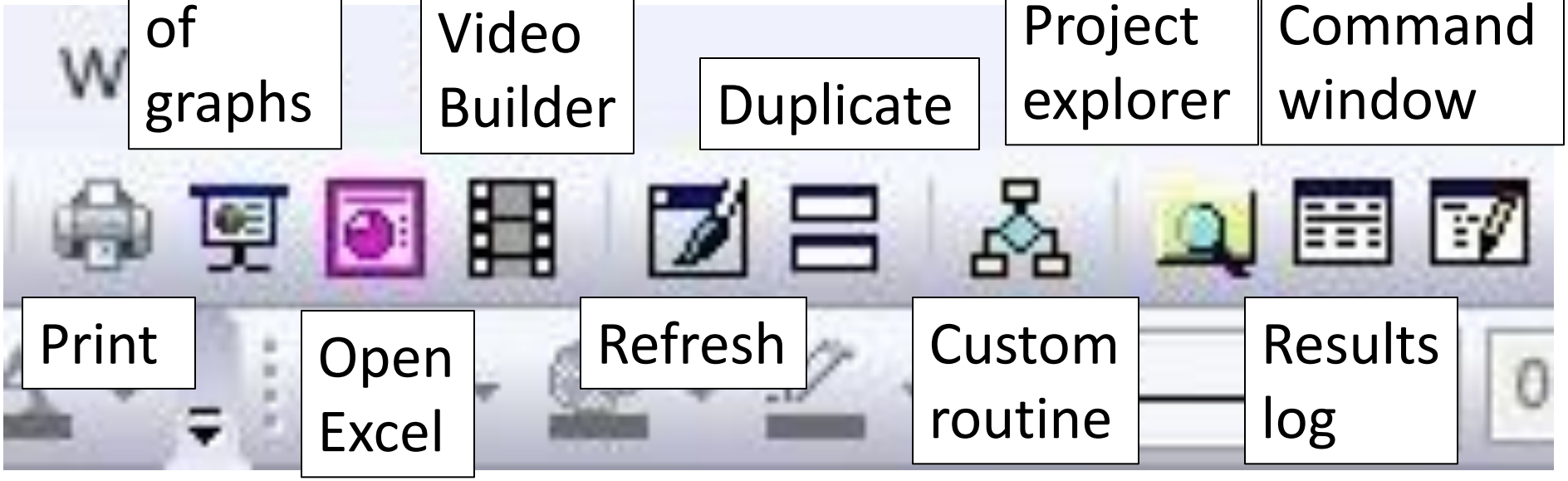
Top Icon Bar: Left



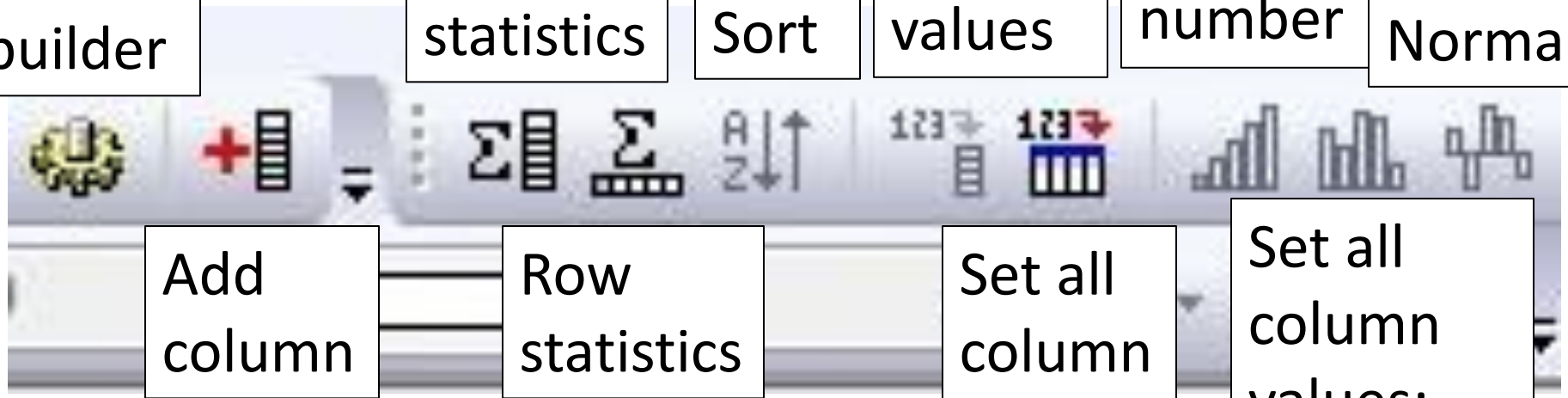
Top Icon Bar: Second from Left



Top Icon Bar: Third from left



Top Icon Bar: Fourth from Left



Code builder

Add column

Column statistics

Row statistics

Sort

Set column values

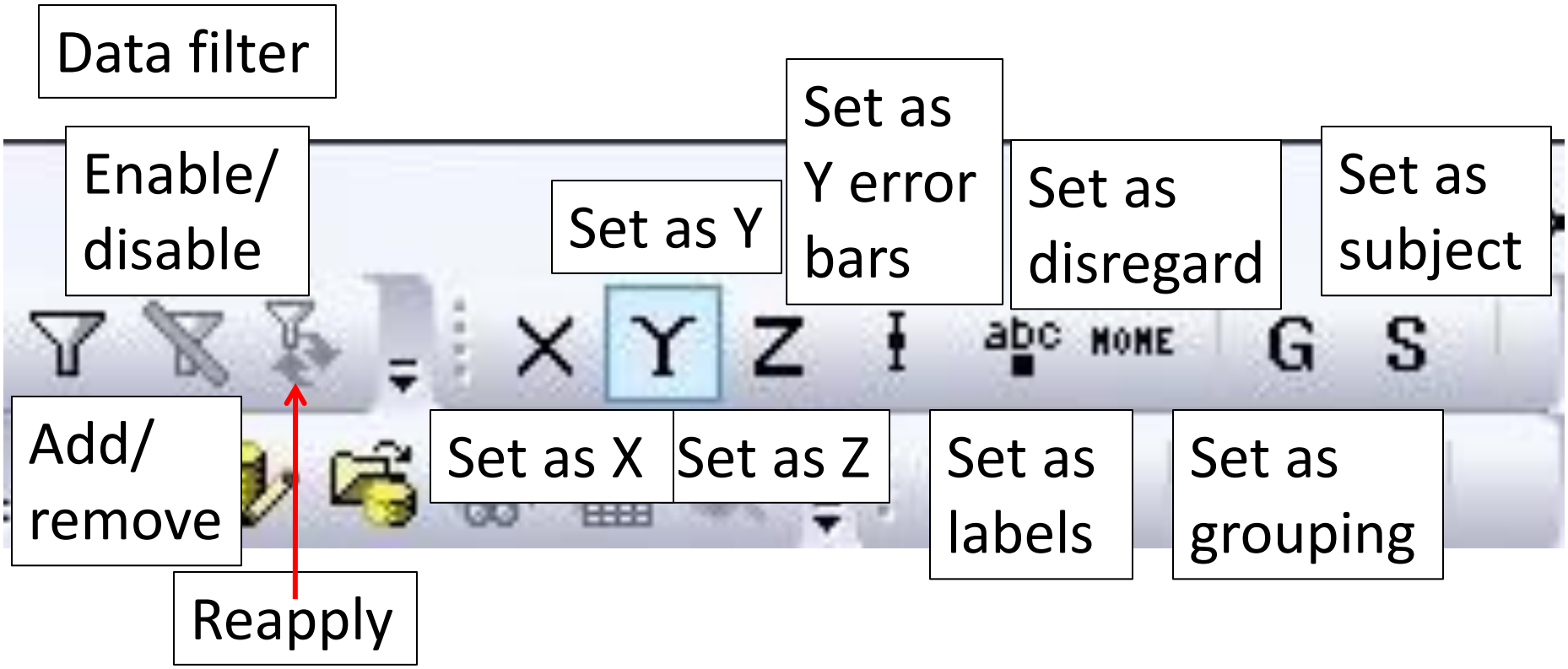
Set all column values

Set all column values from row number

Set all column values: random number

Normal

Top icon Bar: Right



Left Icon Bar: Top

Pointer cursor!

Scale in

Scale out

Screen reader

Data reader

Data selector

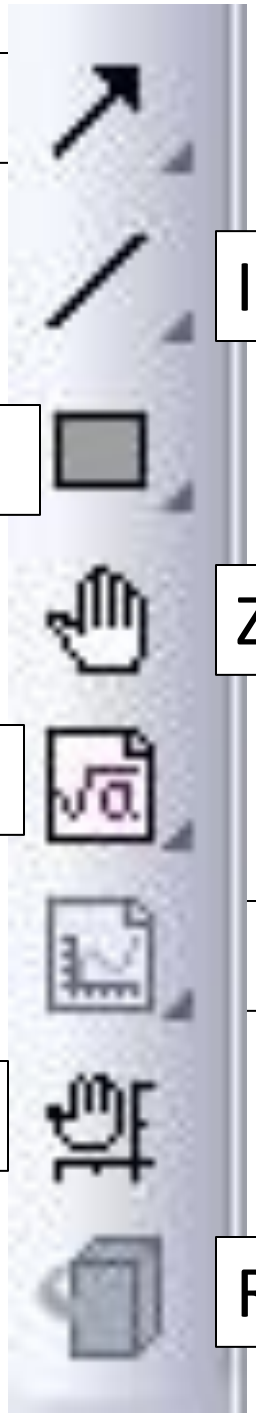
Regional data selector

Regional mask tool

Draw data

Insert text

Left Icon Bar: Bottom



Insert arrow

Insert line

Insert rectangle

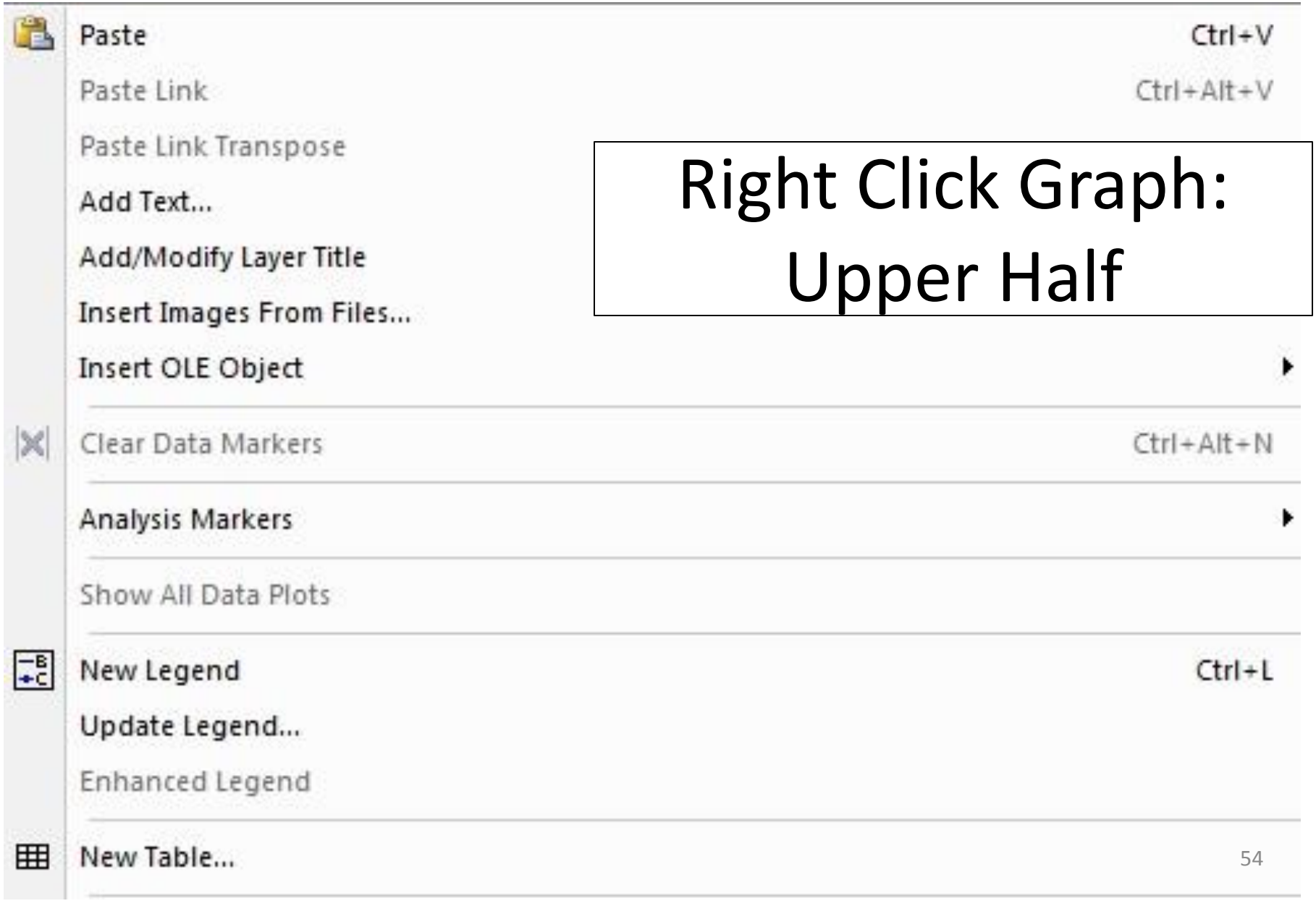
Zoom-panning tool

Insert equation

Insert graph

Rescale tool

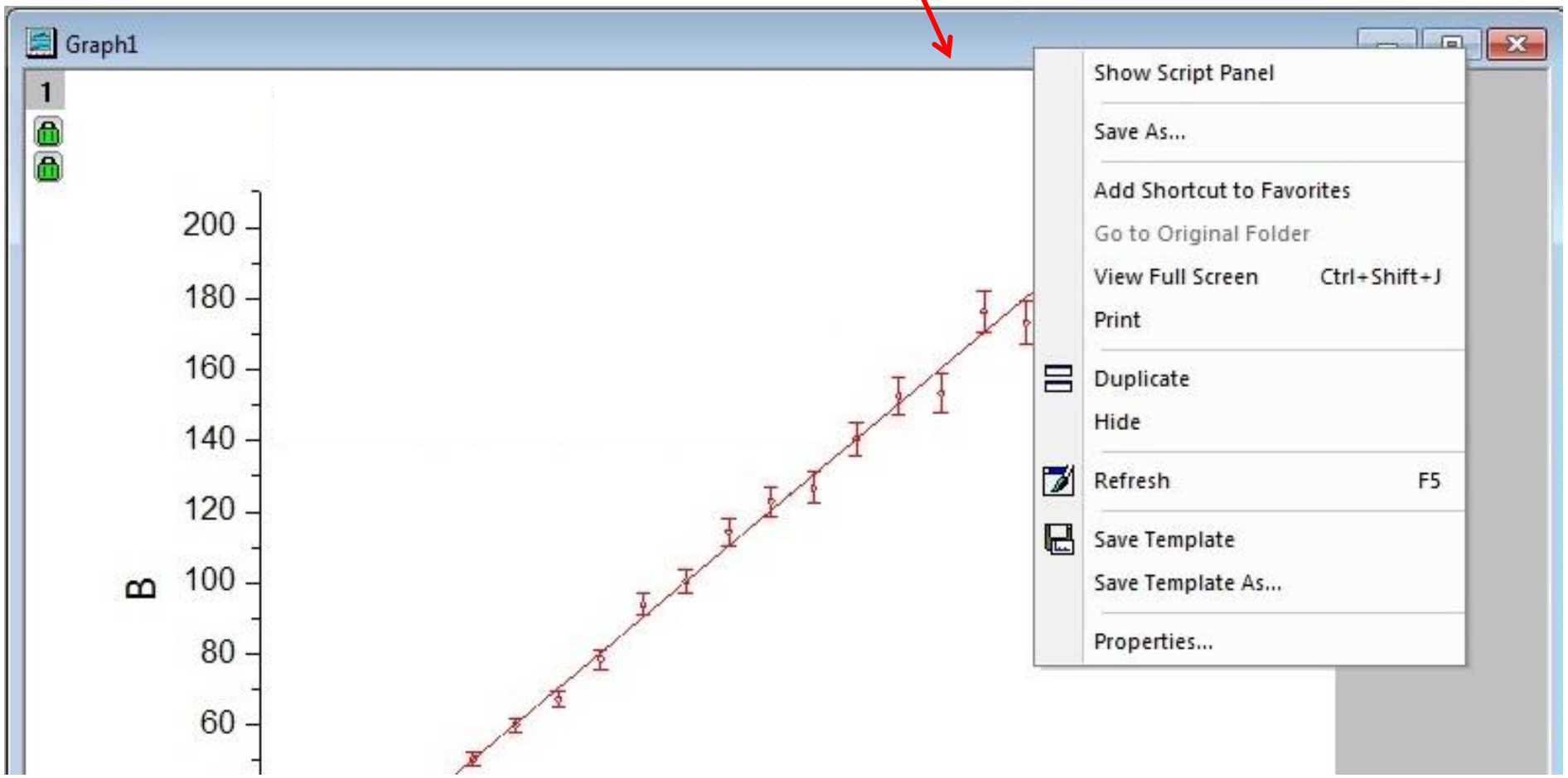
Rotate tool

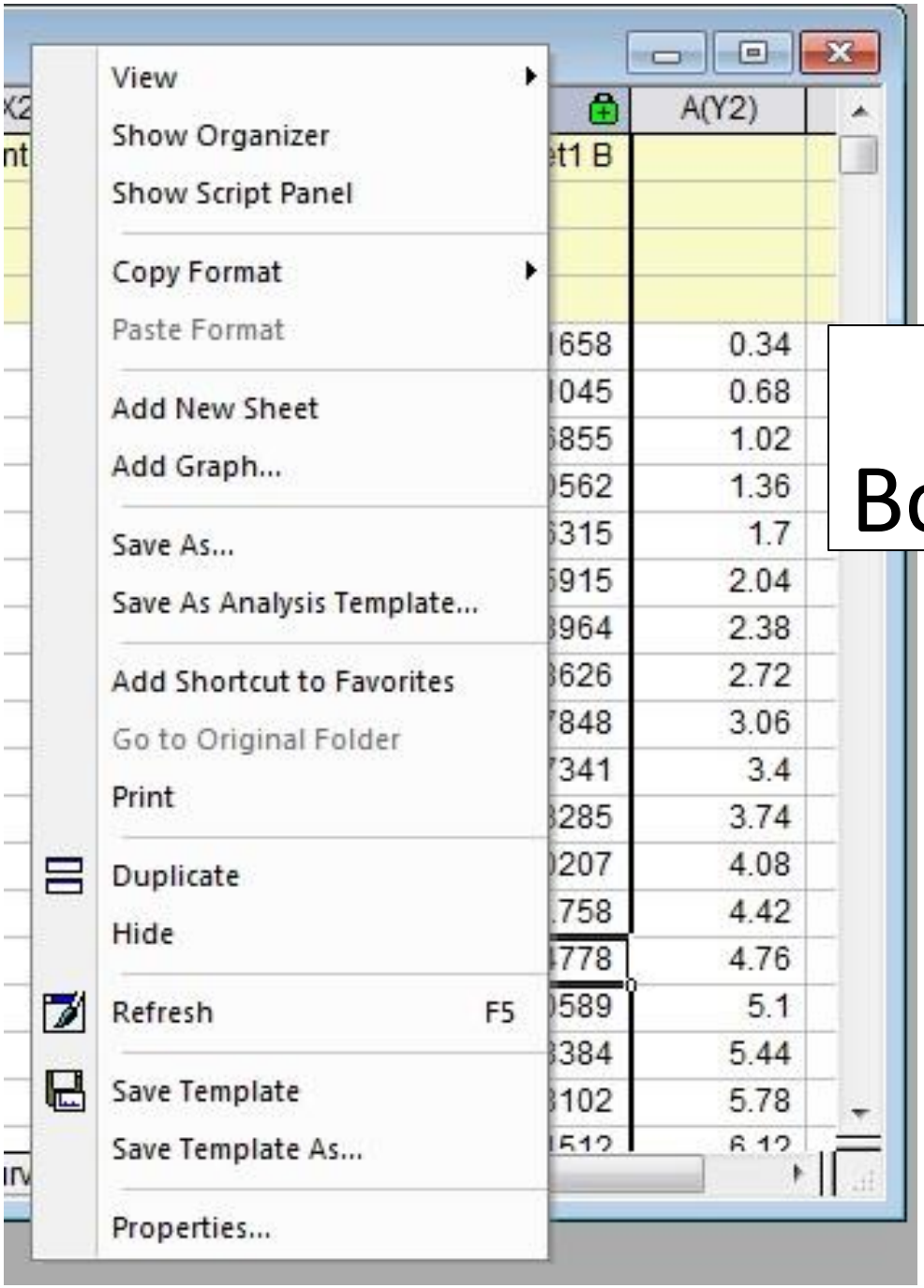


Right Click Graph: Upper Half

Right Click Graph: Lower Half

Right Click Upper Border of Graph





Right Click
Book Upper Border

Miscellany and Minutiae

- Huge amounts of stuff can be accessed by right clicking
  - The menu you get depends on where the cursor is pointed when you right click
- If your graph fills the screen you can reduce it and access the book/worksheet by clicking the expand/contract icon in the upper right
- What else belongs here? Lots!

- To add Greek or other special characters to a text box
  - CTRL M
  - Note that there is only one page of options