Plotting using OriginPro 8.

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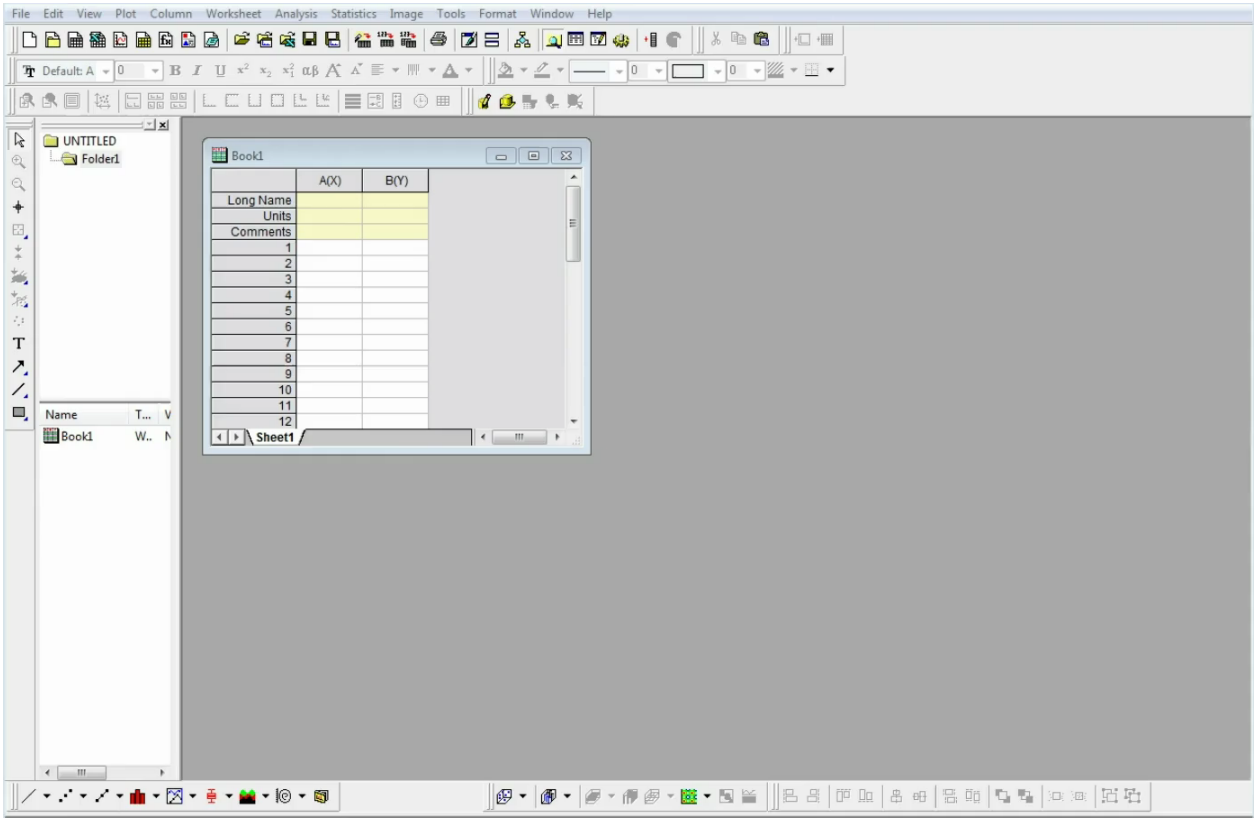
1 Basics of OriginPro 8

OriginPro 8 is a data analysis software that is commonly used to produce publication quality graphs and figures in sciences. This software offers an easy-to use interface for beginner users and ability to customize the analysis and graphing tasks using themes, templates, programming and more for advanced users.

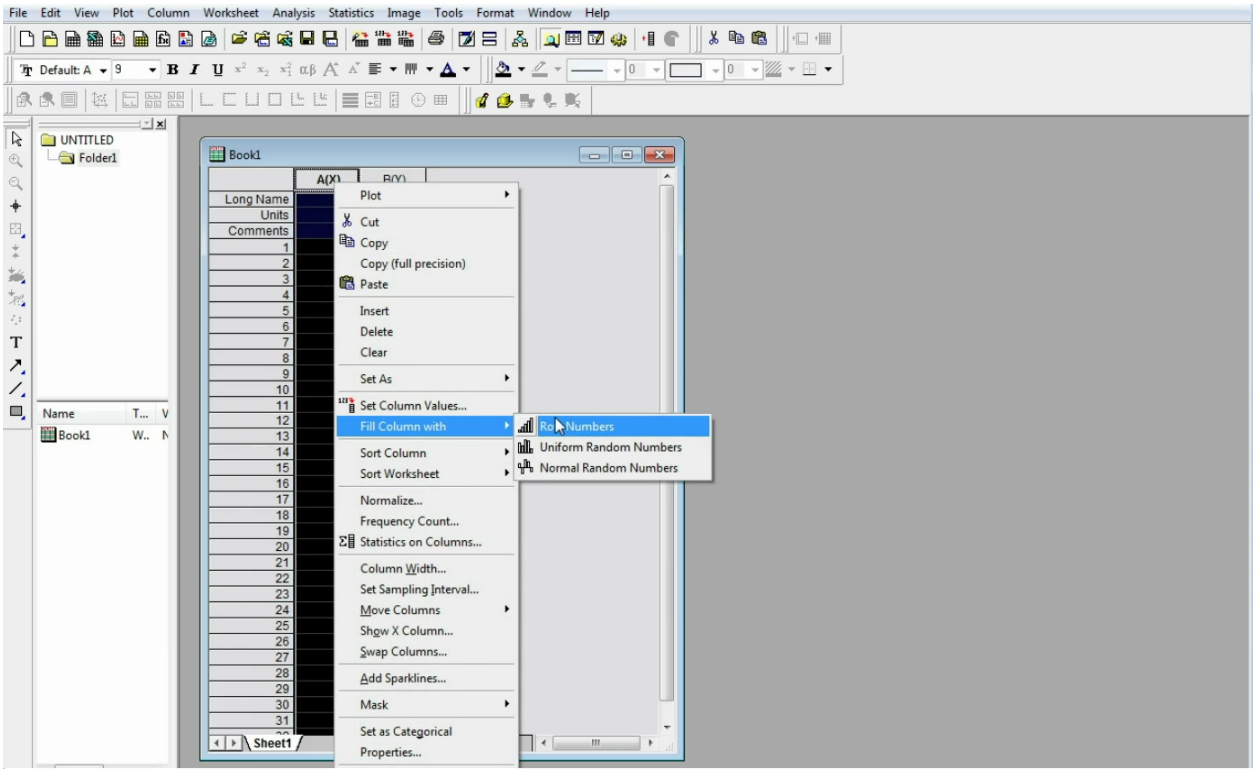


This is the user interface that appears straight away after opening the program. Here you can see a workbook in which your data is going to put and can be analysed.

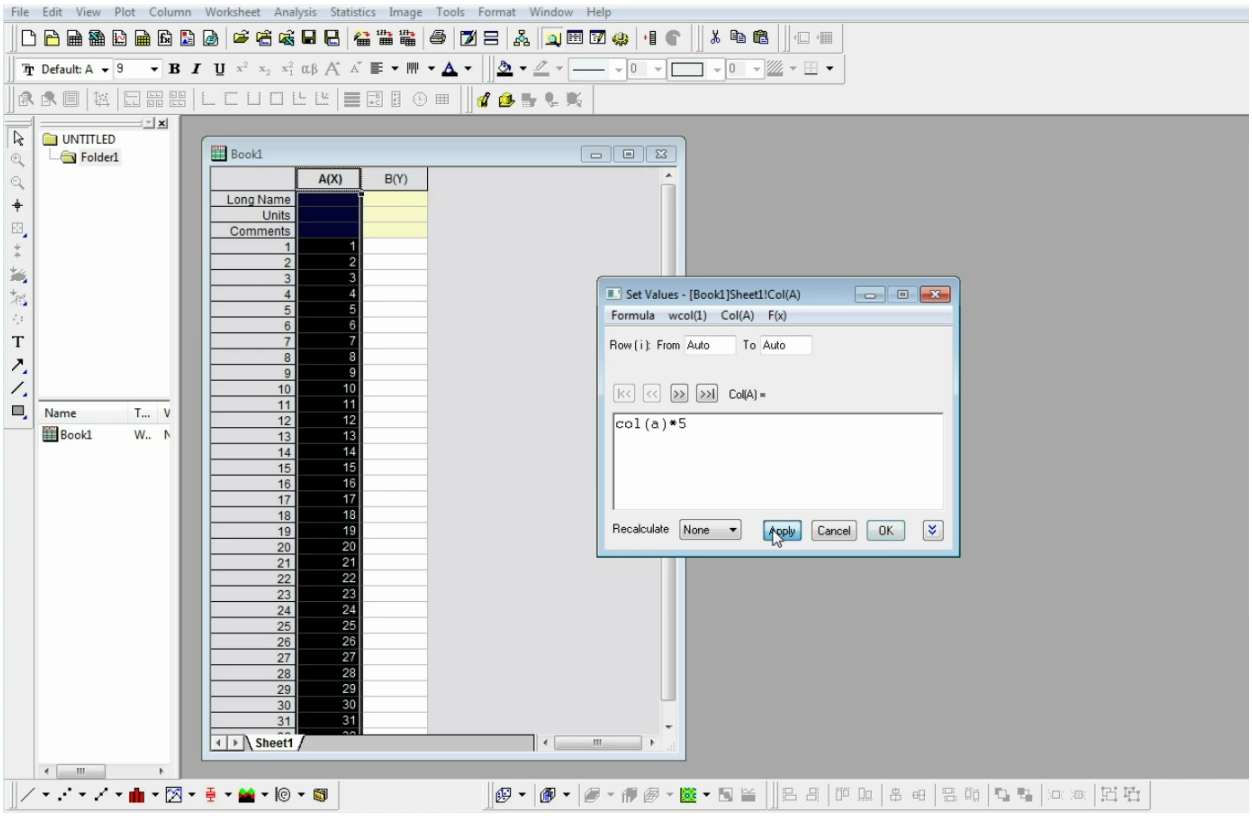
1.1 Input data

By the default, two columns are created. The X or Y the is written after the column name denotes how data is going to be plotted i.e. whether it is going to be X, Y or Z axis' data.

Let's do a quick exercise by creating a simple linear graph. You will need to input data to the columns which will be used to plot the data. Fill the Column A with values that will correspond to our X axis. This can be performed by filling a column with row numbers. This function is accessed by **right clicking on the column**, moving your mouse over **Fill column with** and selecting **Row Numbers**. As you can see this will automatically fill your column with linear increase of numbers.



Moreover, there is another method for when the increments of your x-axis have to be different value than 1. This is performed by **right clicking on your column** and selecting **Set Column Values**

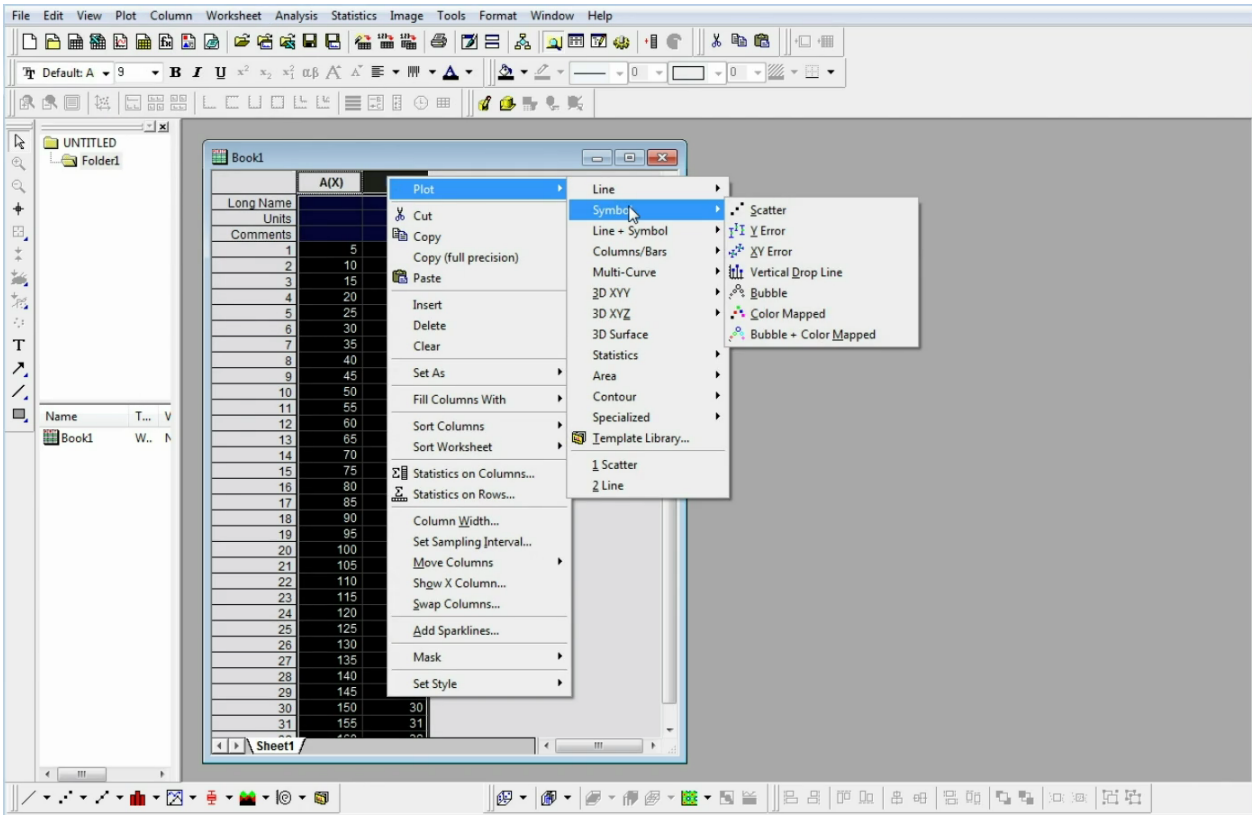


A window will pop-up asking on what calculation should be performed on the column. Here you can see the beginning of your equation $Col(a) =$ and you just have to fill in the right hand side of the equation. As an example, let's make that the step between X-points on our axis is going to be 5. In this case we would write Col(a) = 5*Col(a) and press apply. As you can see, each member of your column A has been multiplied by 5. More advanced and complicated manipulations can be performed in this window. A lot of the functions can be accessed from the F(x). Feel free to explore the F(x) tab for possible functions.

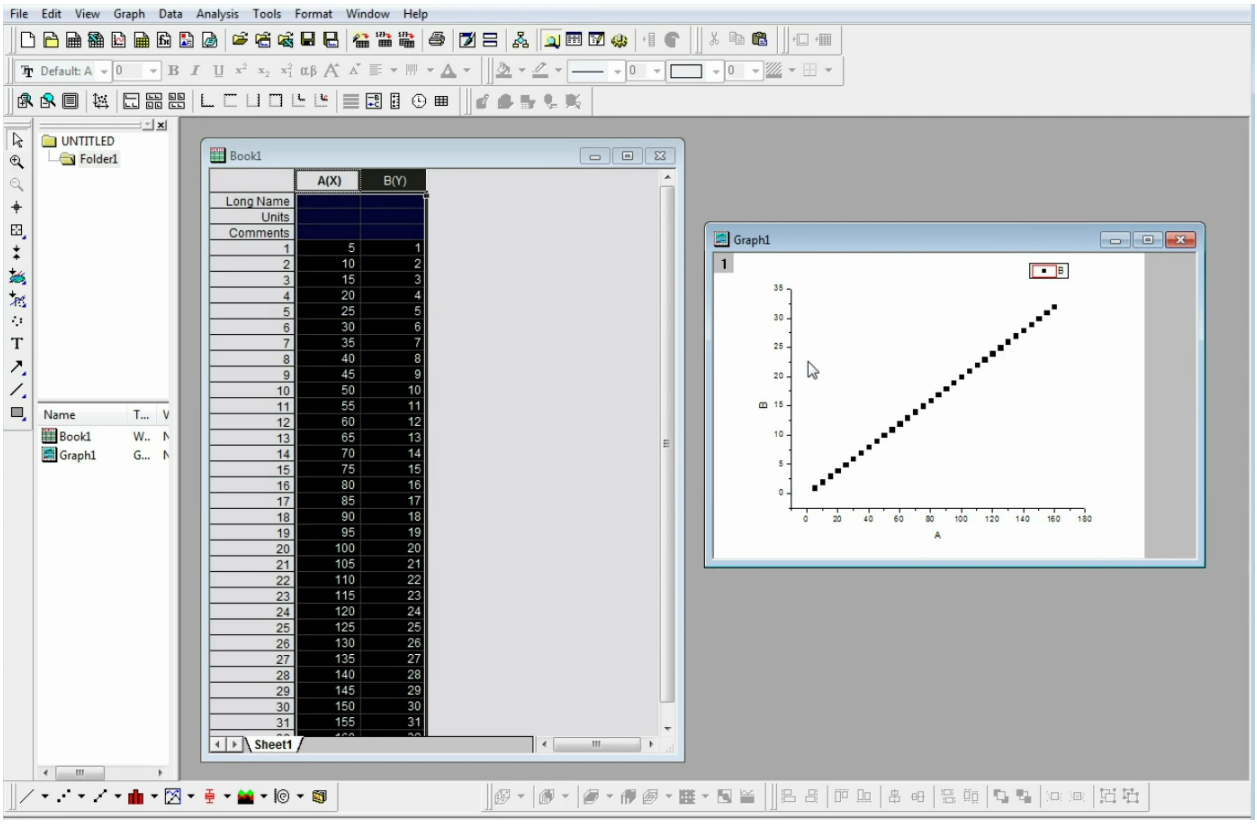
1.2 Plotting a graph

You have learnt how to fill in the data, now try plotting a graph. You will need a Y axis data points for this. Fill in the data as you have done now in column B. Now, plot the data. First, **select the columns** you want to plot by holding the left mouse button and dragging

over the wanted columns. Afterwards, you can press the Plot drop down menu here and select the type of plot you want to your data to be plotted with. As an alternative, you **right click on the selected columns** and **plot** option will appear. This usually a quicker way to plot the data. Let us now **select Symbol** and **Scatter** type.

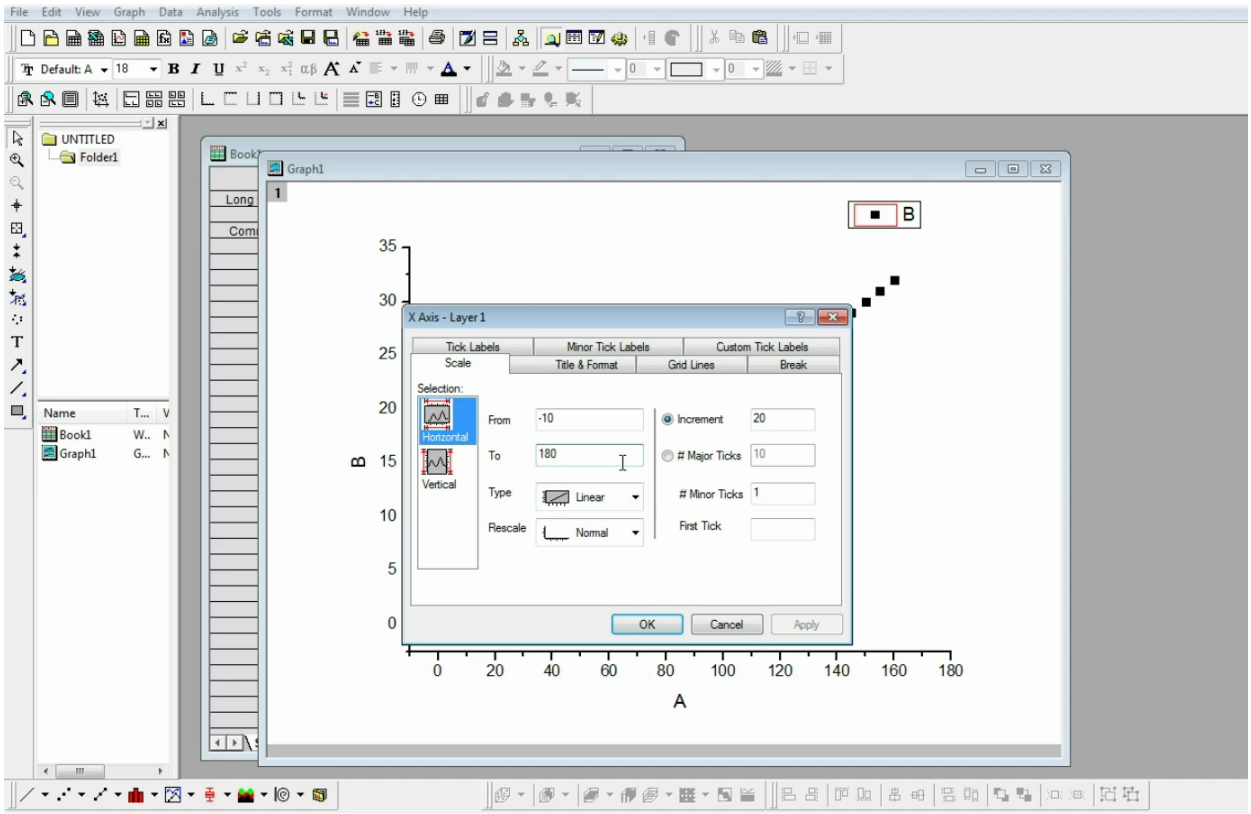


A graph will appear in a different window. As you can see at the top left corner of the graph window and workbook window, they are denoted by different icons. This means that these windows are of different type. For example, if you will select the graph window, the options at the top will change to ones applicable to a graph rather than the ones needed for a workbook as you can see now.

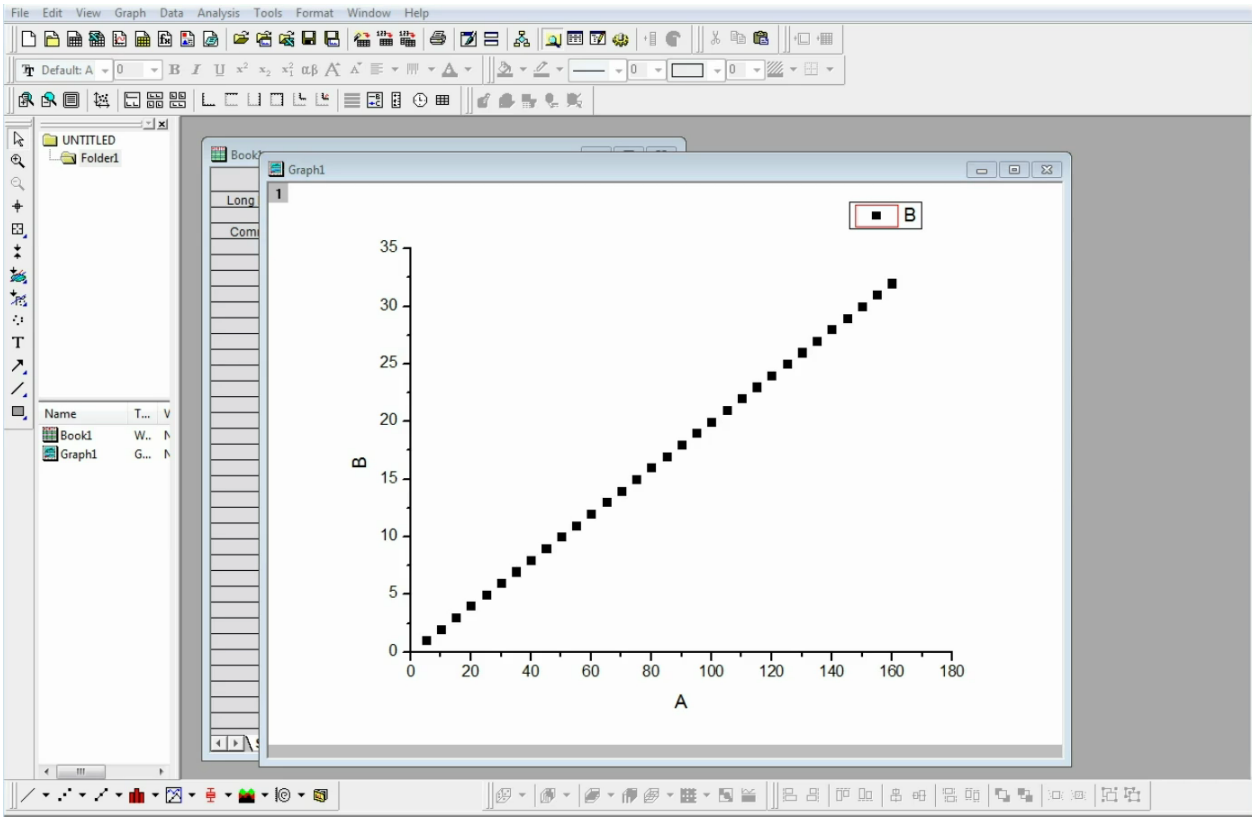


1.3 Manipulating your plot

Time to perform basic manipulations on the graph. First, adjust the axes so they start at 0 rather than at a negative value. This is done by **double clicking on the axis** and an "X axis" window will appear. Many parameters can be changed here. For example, where you want your axis to be positioned, what font to use, adjust your ticks on the axis and more. Please feel free to explore the options available. We will focus on the **scale tab** here. Here you can select the range "from" and "to" as well as type, increments and tick values. I find this to be the most commonly used tab of this window. So, we want our X-axis to start at 0. It is starting at -10 now. Change this value to 0 and click apply to see the change. Click "OK" to close the window. Let us perform the same change on Y axis as well. Double click on the axis, select "Scale" tab, and change the value from -2.5 to 0.

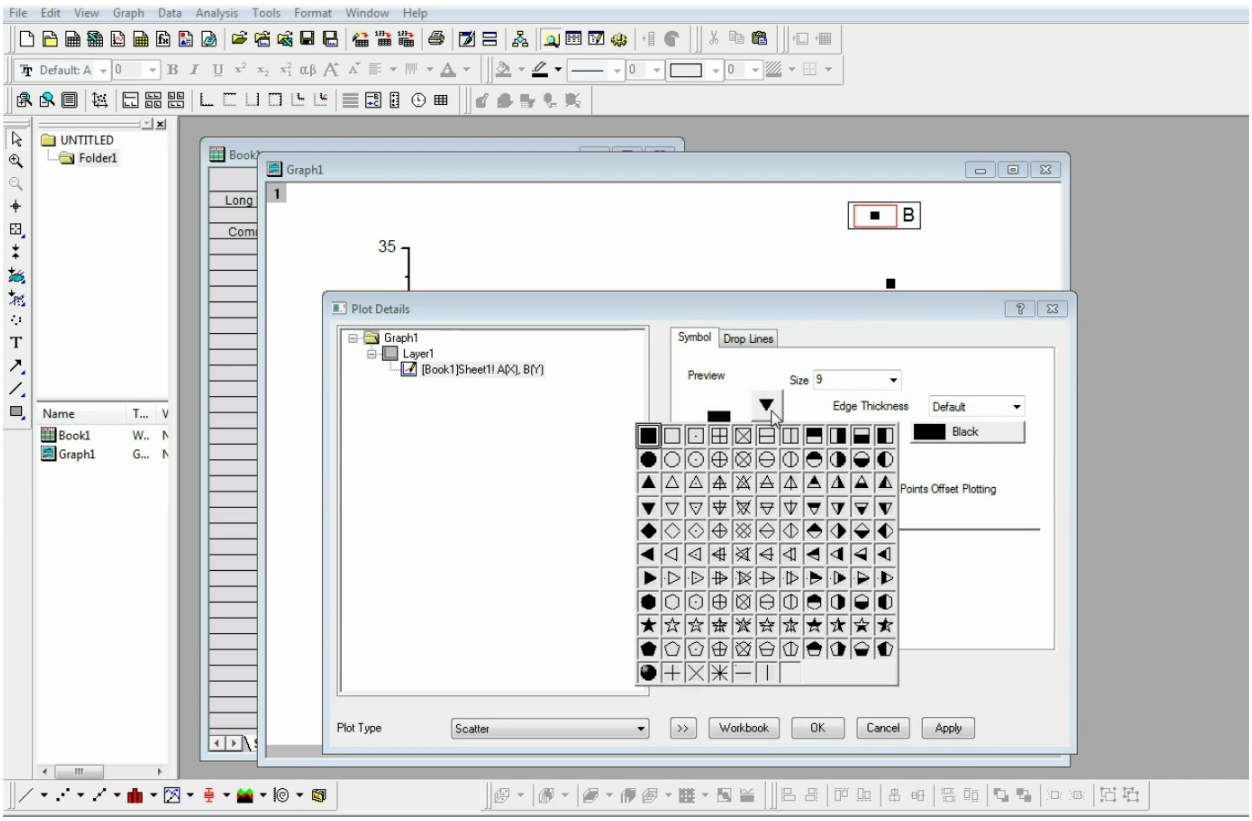


It is important to mention, that the changes made on the graph do not alter the data in your notebook. As you will see later, analysis operations performed on your graph will create new tabs in your workbook with the data corresponding to the analysis performed.

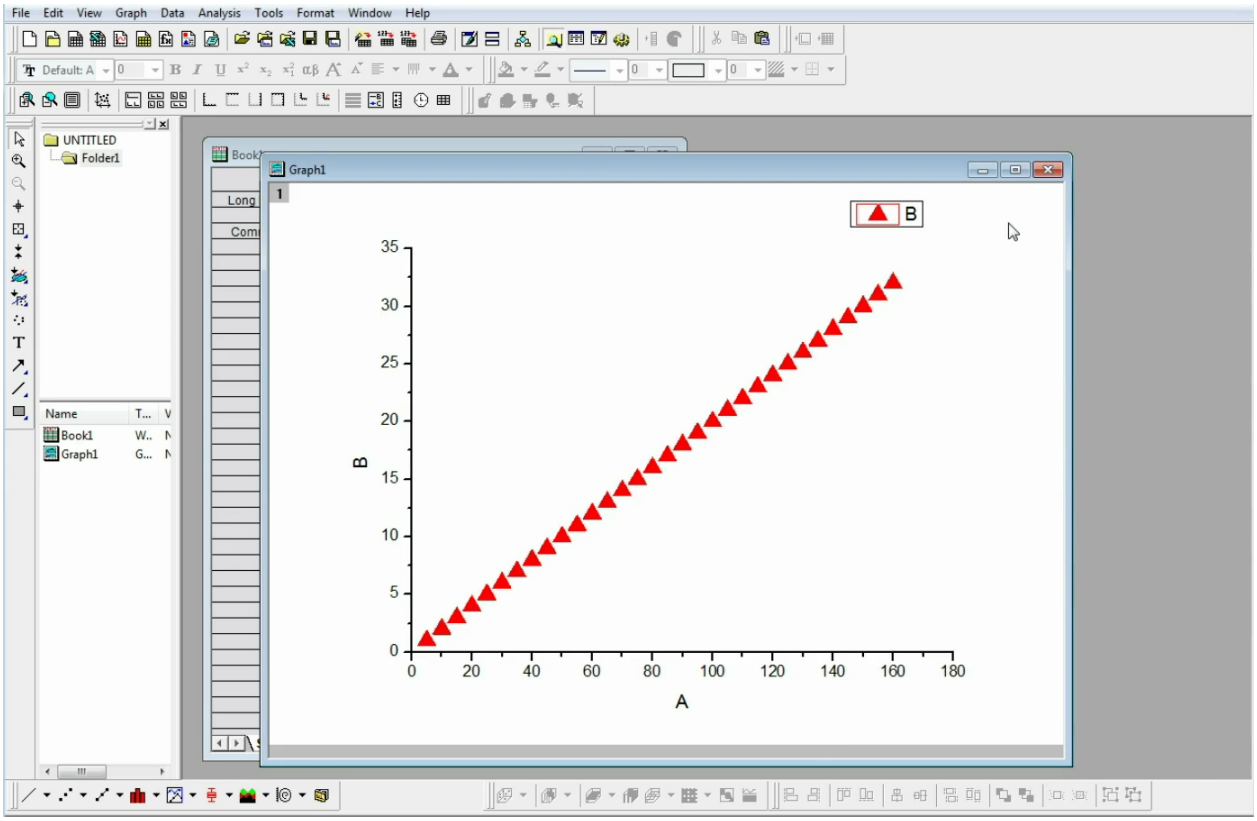


1.4 Manipulate the way the data is presented

Now, manipulate the way the data is shown. **Double click on the data points**. A **Plot Details** window will appear. On the left hand side is the reference to where the data for this plot is taken from. On the right hand side, you can manipulate on how you want the data to be presented. Here you can adjust the size of the data points, the shape it is represented by, the color and more. Pressing "Show construction" allows you to manually generate on what shape should be used for representing the data. However, the suggested shapes from this drop-down menu is more than enough.

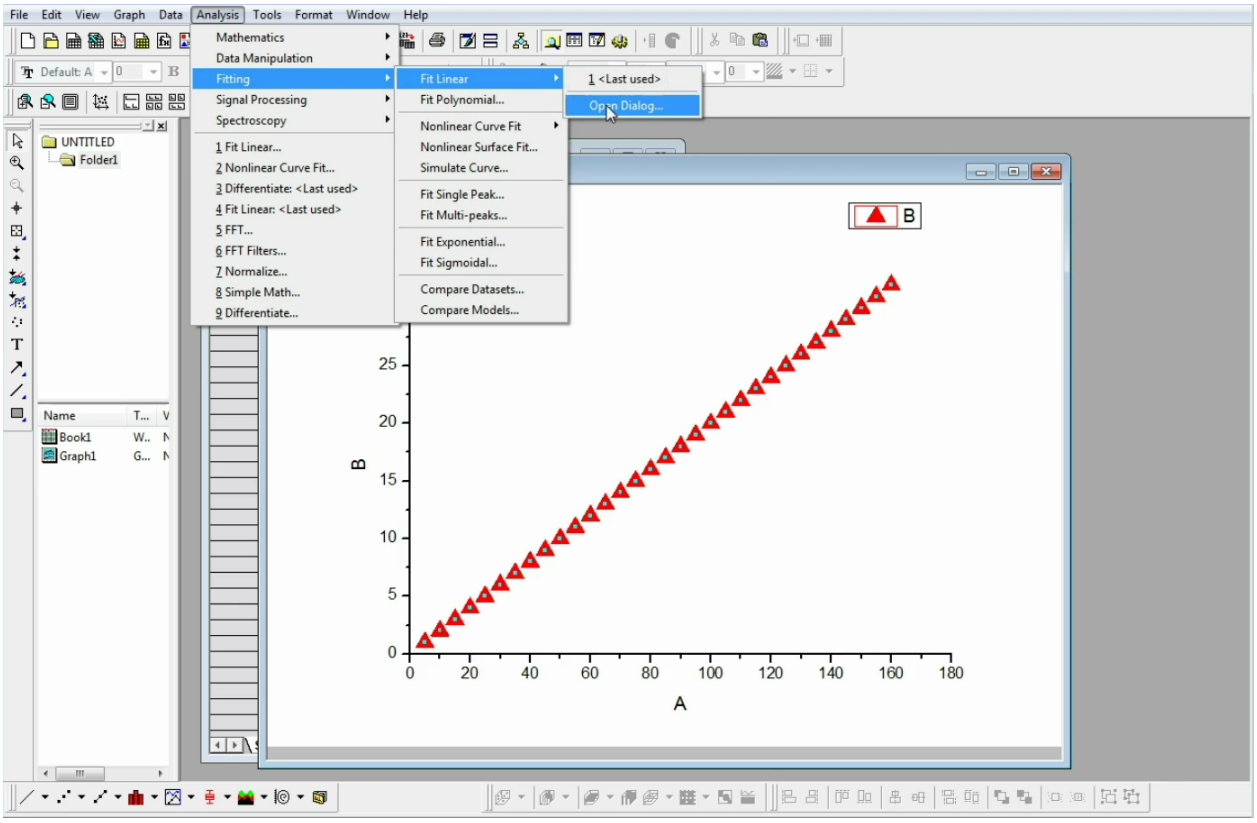


So, as an exercise, change the shape of the data to a triangle by pressing the drop-down menu and selecting a triangle shape, increase the size to 12 and change to color to red. Press "OK" to apply the changes.

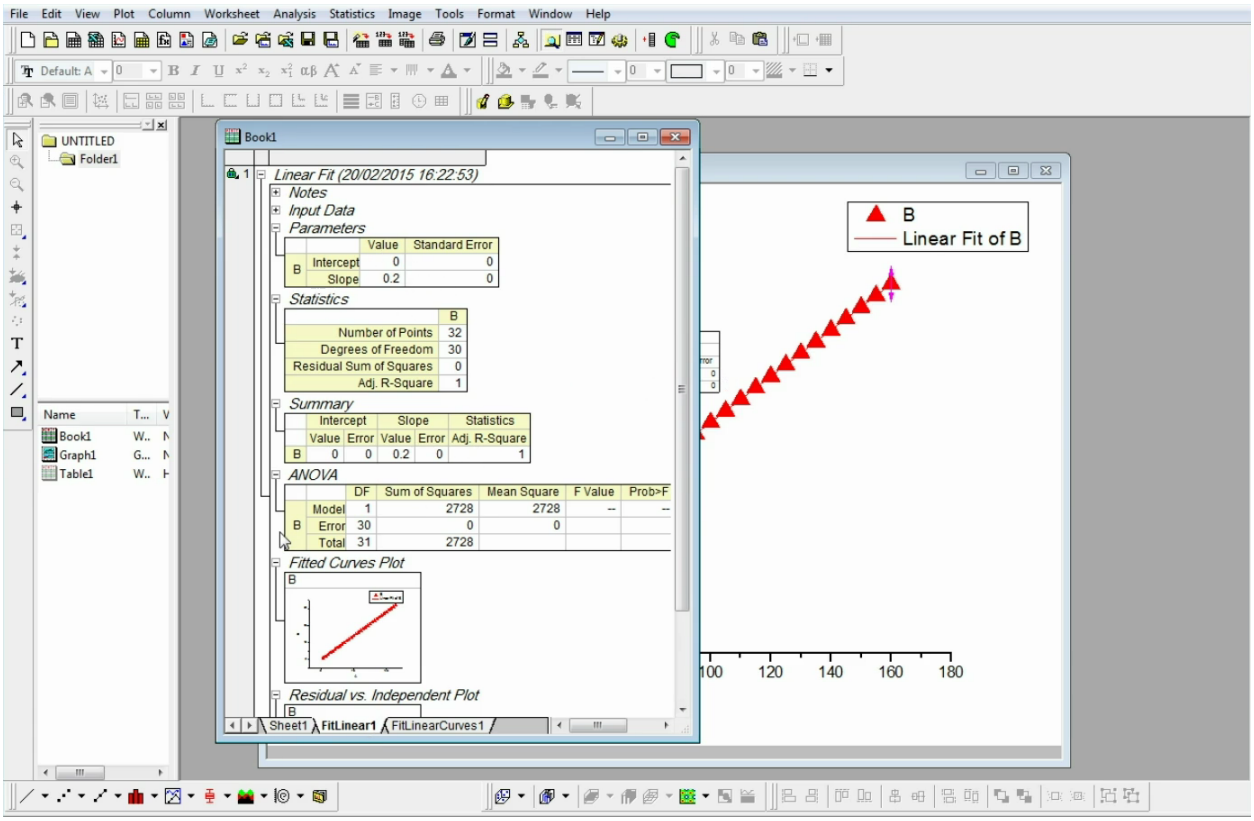


1.5 Fitting the data

After you have learnt how to plot data and manipulate the graph you can try fitting the data. The data is fitted by **selecting your data points using the left mouse button**. Afterwards, **select "Analysis" tab** from the menus at the top and **select fitting**. As you can see here are many different types of fit such as linear, polynomial, non-linear curve and others. Let us select "fit linear" for our data.



A Linear fit window will pop up. Here you adjust the parameters you want your fit to have but for this exercise we will keep it basic. Press "OK" in order to apply the linear fit. A window asking for a report sheet will come up. Select yes as this report sheet contains the quantitative information of your fit. This is generated in the same workbook that the data comes from but a new sheet is created to contain the information from the fit. FitLinear1 sheet contains information about the fitting such as intercept points, slope, degrees of freedom and others. This will contain the useful information you want to extract by fitting any type of data. If you want access the raw data of the fitting line itself select the FitLinearCurves1 sheet. Here you can see the fitting line's raw data, the residuals and others. This is useful when you want to do manipulation on the fitted line.



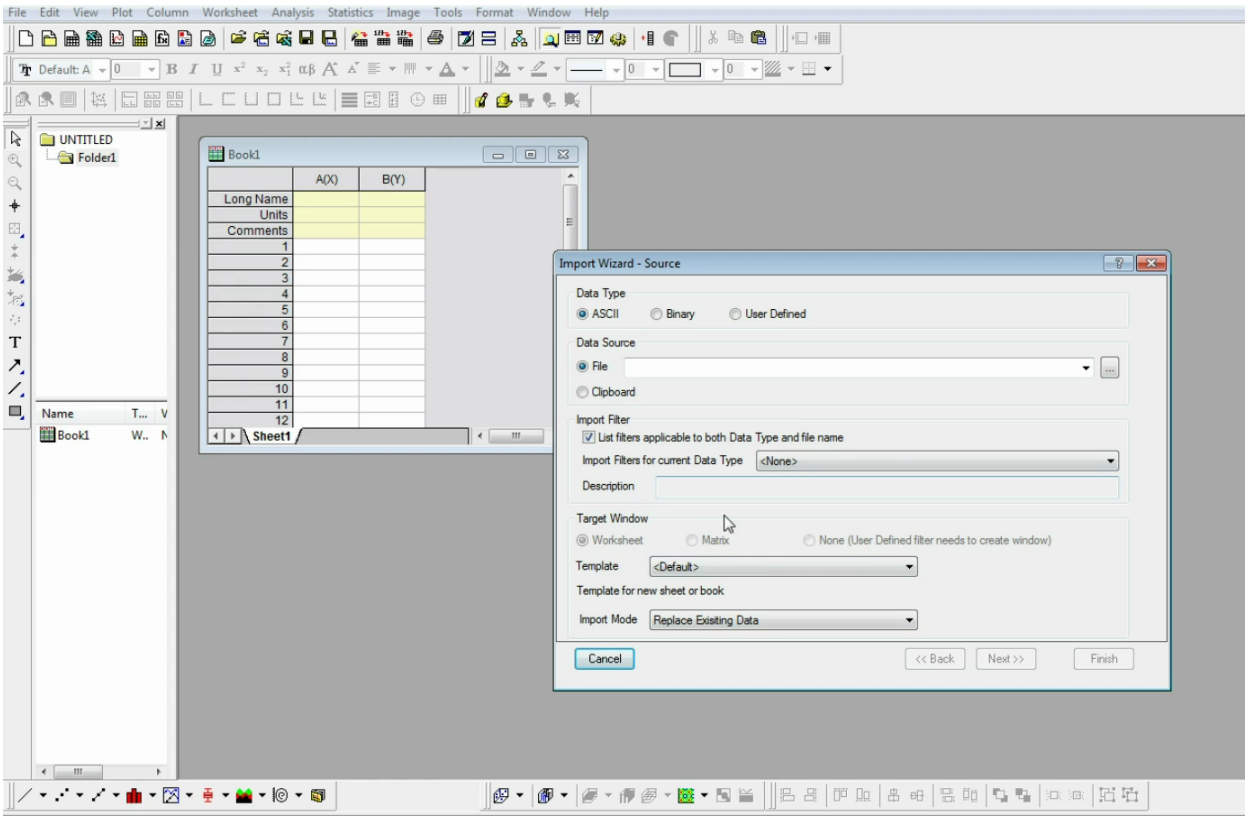
2 Exercise: Fitting multiple Gaussian peaks

This exercise will put all the things you have learnt so far to the test. For this exercise a file with data will be provided that contains a spectrum with two Fe55 peaks. The aim of this exercise is to plot the data, fit two Gaussian peaks on the same graph, extract sigmas with errors and make the graph into a publishing quality figure.

2.1 Importing data

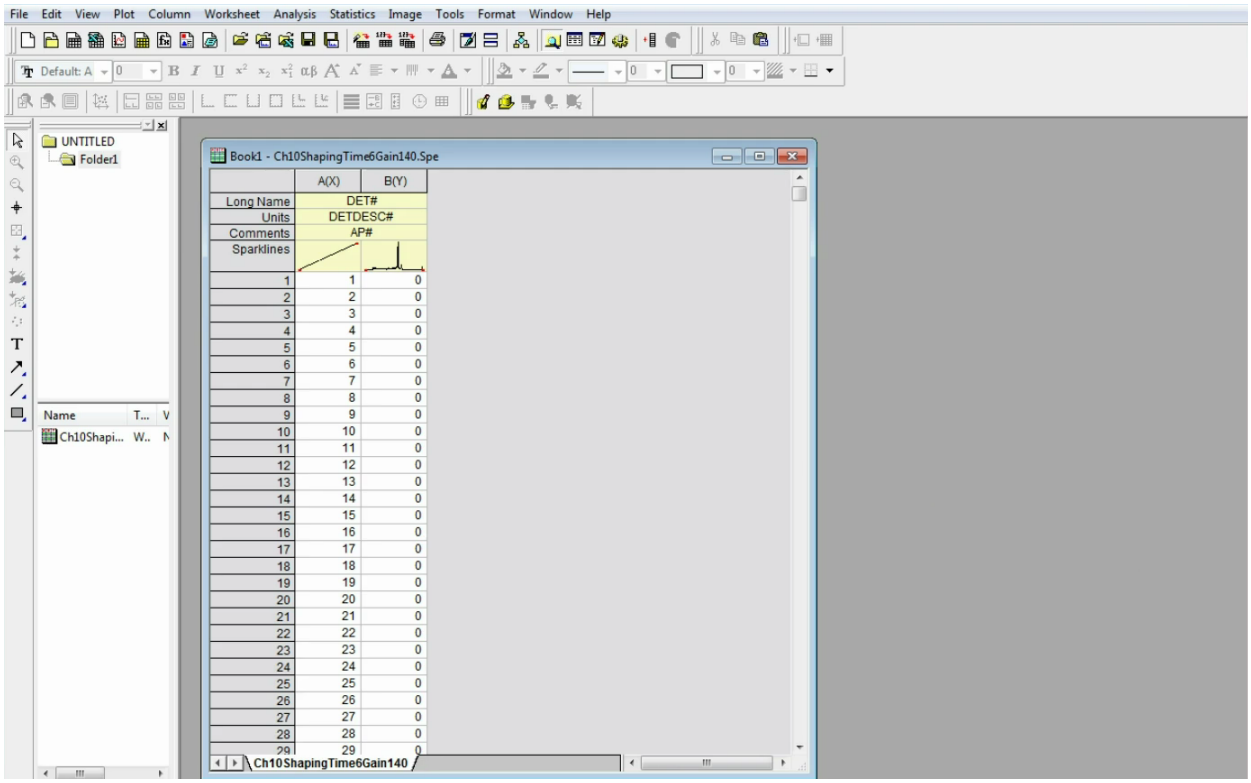
To begin, open a new project in your OriginPro8. You should see only a workbook 1 appearing . Now let us import the data. OriginPro8 has a great import wizard that allows you to import data from many different types of files. The file you downloaded should be in .spe format. In order to import the file, **press File, Import, Import Wizard**. If import

options is not there, make sure you have your workbook window selected. In this window, you can select a type of data your file is in whether it is an ASCII or Binary. Press on the right hand side of File, the "..." symbol to open an import window. Select the file and press add files. Using this window you can also import many data sets on one go. Press OK to close this window and press Finish.

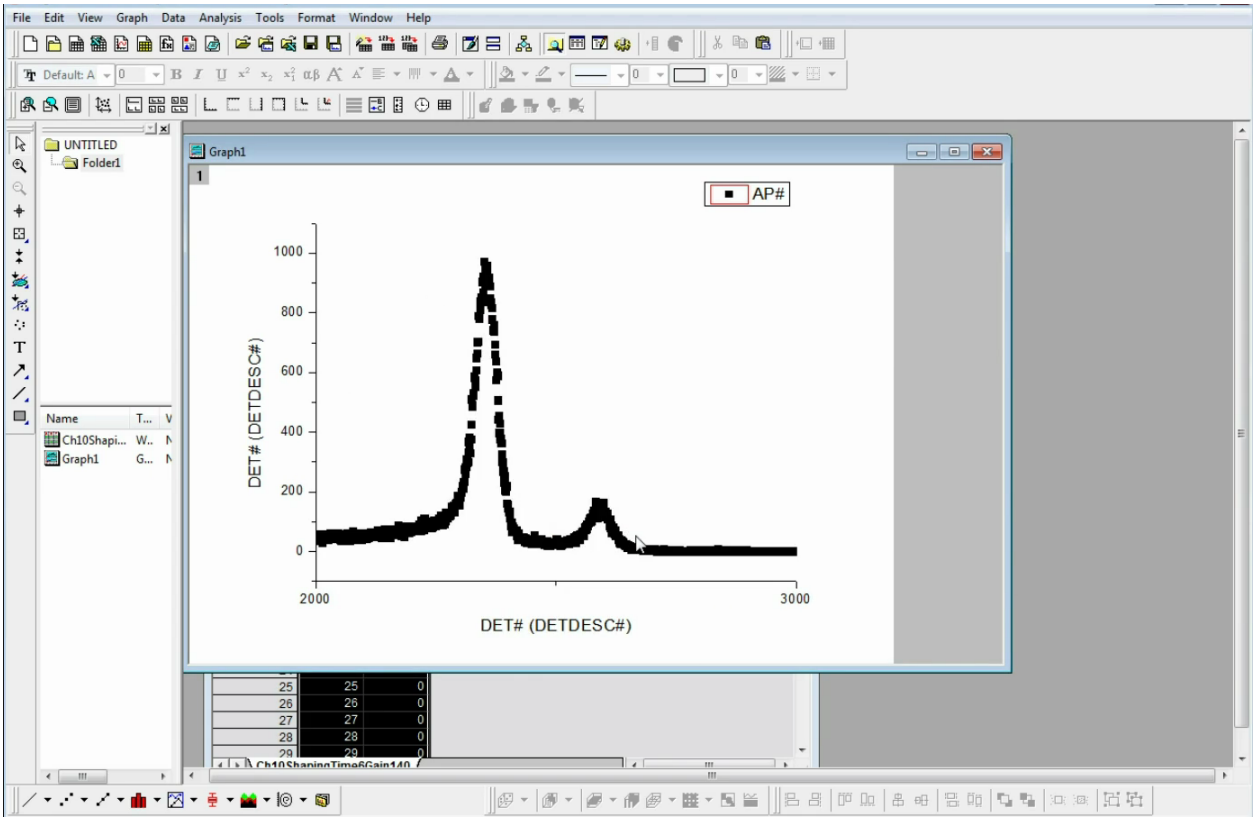


2.2 Plotting the data

Our data is now imported into our workbook. Column A contains the data we need for the spectrum while column B contains channel information which holds no value here. Copy the data from Column A to Column B because you want this data set to be on the Y axis. In order to generate X axis data, Right click on the column A, Fill Column with, Row numbers.

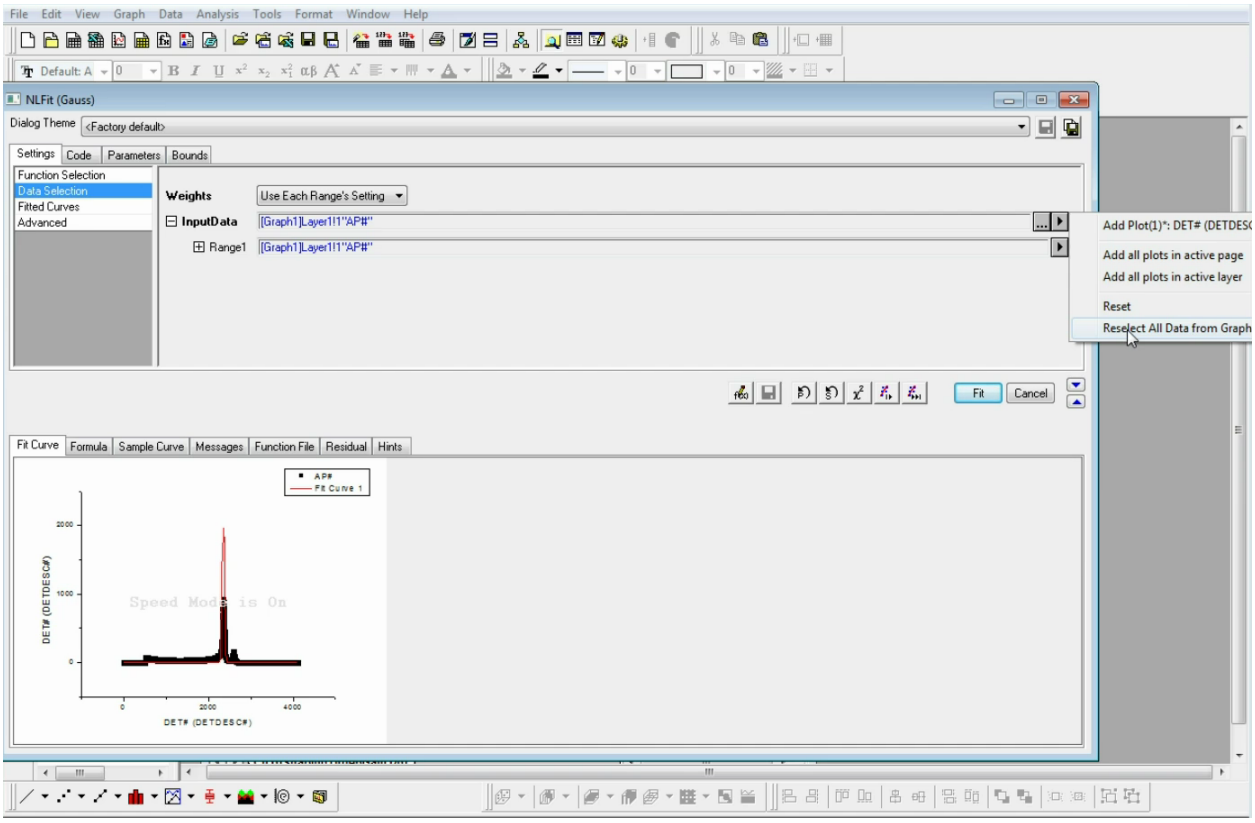


Your data is ready for plotting. Select both columns, right click on them, plot, symbol, scatter. Here we have our spectrum plotted. You are interested in the two peaks in the middle of the plot. Zoom in onto them. Double click on the X axis, Scale, and change the range to be 1500 to 3000 and press OK. No we have a much clearer view of our plot. Also, sort out Y axis as well because negative values are of no interest. Double click on Y axis, Scale, Set lower range limit to 0.

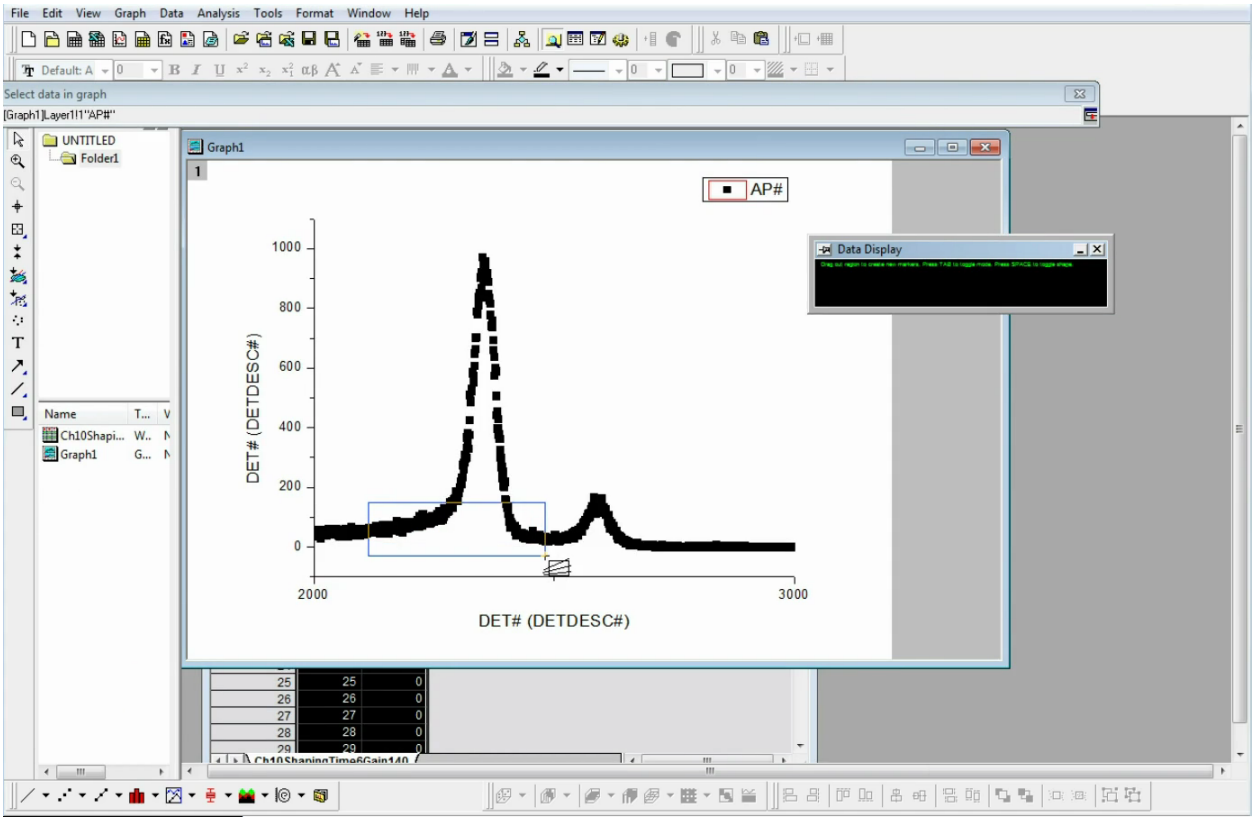


2.3 Fitting the double Gaussian onto the data

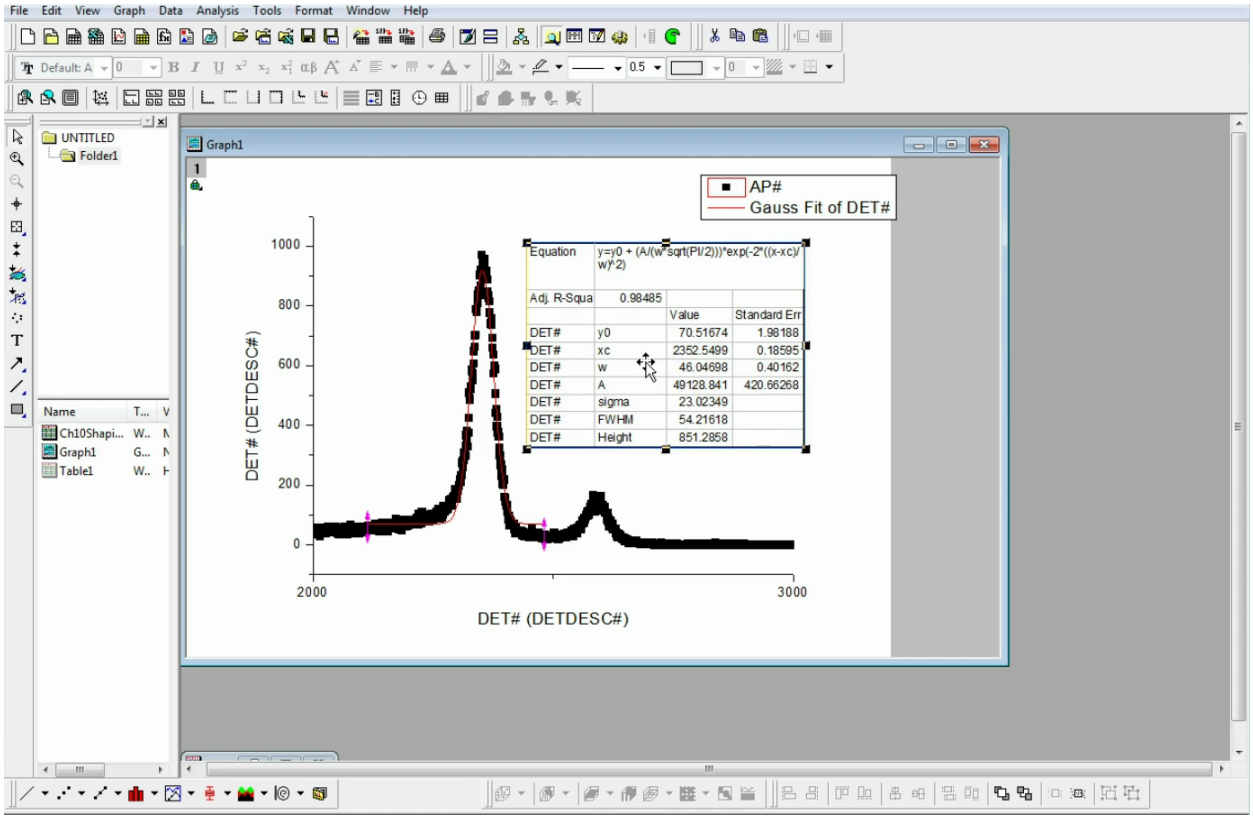
Here we have to peaks and we want to find out what width they are. For this we can use Gaussian fitting and extract standard deviation or sigma out of it. To do this **press on the data points, "Analysis" from the menu, Fitting, Non Linear Curve fit, Open Dialog**. In this window you can select what type of non linear curve fitting function to fit your data with. In category, you can find various types of fitting functions such as basic, exponential, logarithmic and more. You are interested in Gaussian function, which is under Origin Basic Functions and called Gauss. Now, fit every peak independently. For this, go to **Data Selection** menu, press the **arrow on the right hand side of the InputData and Reselect all data from graph**. This allows you to select a region to fit.



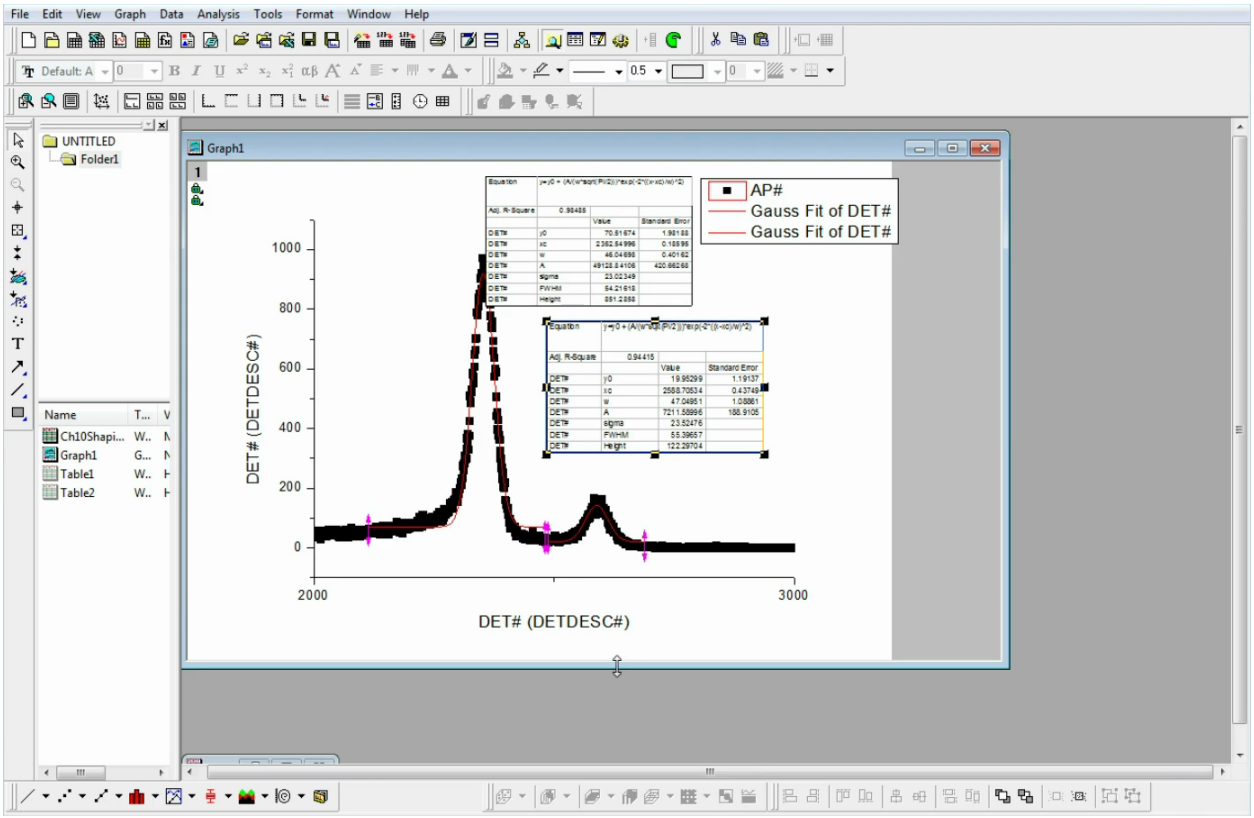
Now select an area around the first peak on the icon on the right hand side of the "Select data in graph" window. The region should be selected and return you to the original "NLFit" window.



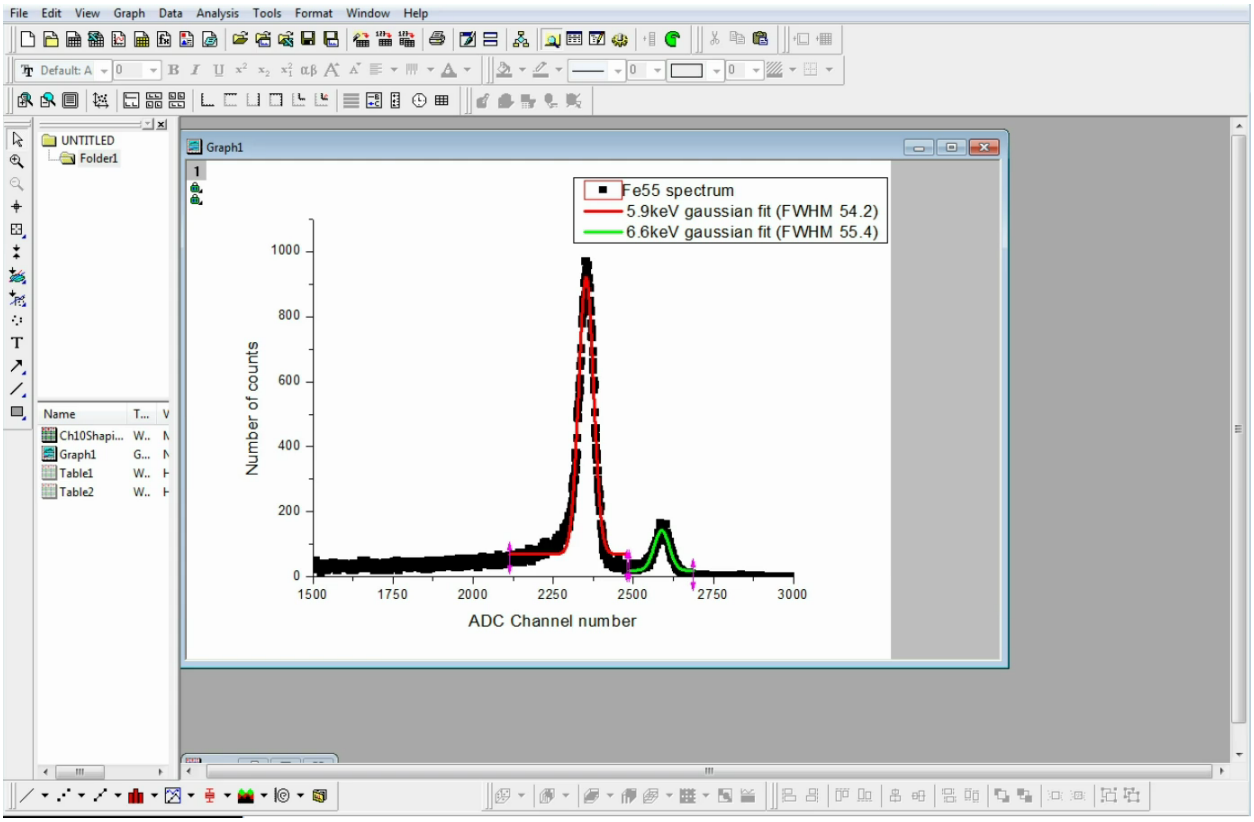
Press Fit. Again, ask for the report sheet. Also, a table next to your graph should appear with the main parameters extracted from your fitting function. It shows what equation was used to fit the data and values for each parameter extracted.



Now repeat the same for the second peak. Analysis, fitting, Non linear curve fitting, Open Dialog. Data selection, Reselect Data from graph. Select region around the second peak. Press fit. The second peak is now fitted as well. A second table with parameters is generated.



Finally, tidy up the graph. Change the X-axis label to “ADC Channel Number“ by double clicking on the label. Change Y axis label to “Number of Counts“ by double clicking on the label. Also, the ticks on the x axis are too sparse. Make the increments smaller. Double click on the axis, scale, Increment is set to 1000. Change it to 250. Since you have fitted two peaks, let us change the color of the curves. Double click on the curve, change color to green and increase width to 3. For the first peak just increase the width to 3. This way our fits of the peaks are clearly visible. Now adjust the legend to explain what everything represents. Our data is an Fe55 Spectrum. Red is the Gauss Fit and let us include the sigma value in the legend as well. Same goes for the green fit. In order to finalise our graph, delete the tables. Also, you could adjust the x axis to zoom in so that even less “empty space“ is visible. Change scale from 2000 to 2750 and increments to 100. A publication grade figure is produced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6.6keV gaussian fit (FWHM 55.4)
Number of counts
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1750
2000
2250
2500
2750
3000