Magnetism Reflectometer
Data Reduction Manual

Revised 5/10/2007

A U.S. Department of Energy Multilaboratory Project

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Magnetism Reflectometer
Data Reduction Manual

F. R. Klose
H. Ambaye
R. J. Goyette

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Prepared by
OAK RIDGE NATIONAL LABORATORY
P.O. Box 2008
Oak Ridge, Tennessee 37831-6285
Managed by
UT-Battelle, LLC
for the
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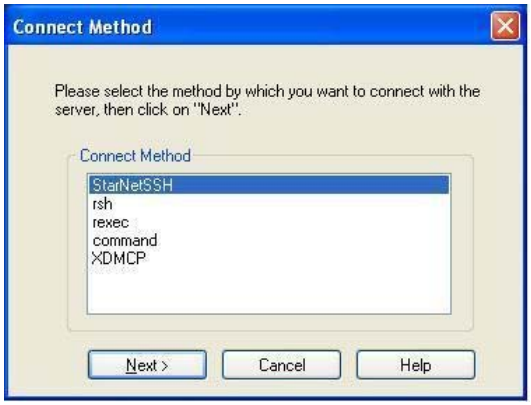
Magnetism Reflectometer Data Reduction Manual

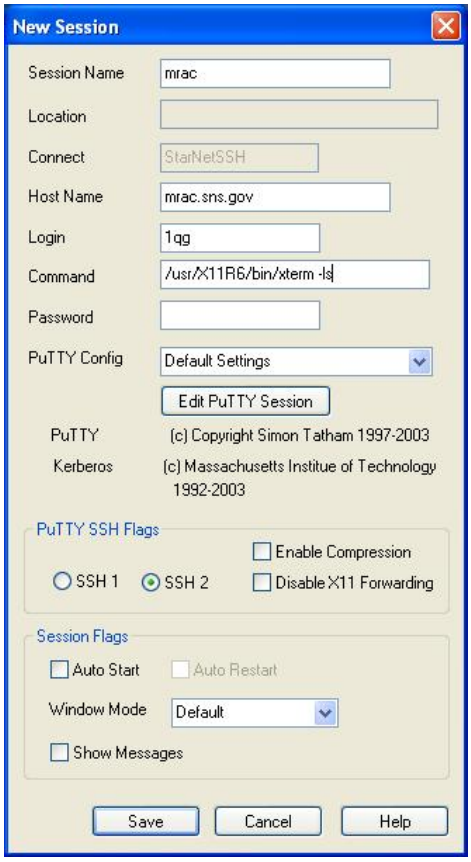
Data reduction on the Magnetism Reflectometer begins by connecting to the analysis computer mrac.sns.gov using software that supports *X-Windows* connections via the *SSH* port (port 22), also known as *X11 tunneling*. On a system with *XWin-32* installed, start the application from the **start menu**:

The *X-Win32* logo will appear on the menu bar at the bottom of the screen. Right click on it and select **XConfig**:

Click the Add button to configure a new session. You will be asked what type of connection type you want. Select **StarNetSSH**:



Then fill in the rest of the session information:

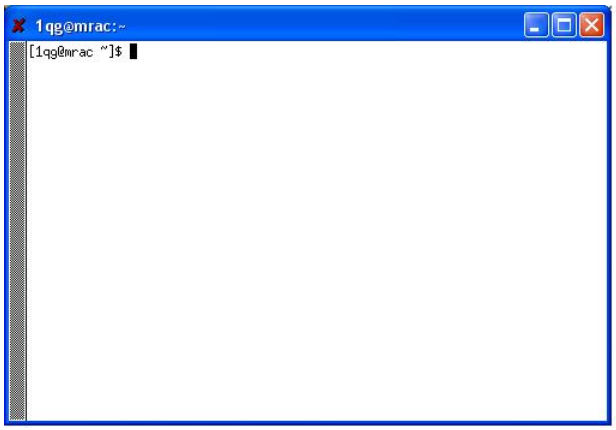


The session name can be anything you want. The host name should be **mrac.sns.gov**. The login should be your **XCAMS** username. The command should be **/usr/X11R6/bin/xterm –ls**. Click **Save** when you are done. The session is now ready to use. Click on the *X-Win32* logo in the menu bar again, and select the session you just created:

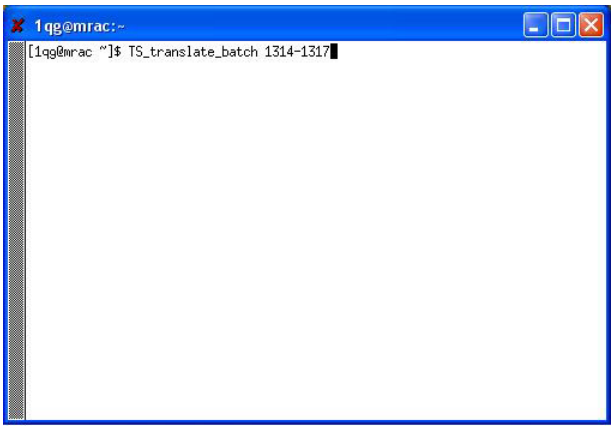
Then enter your username and password information:

If this is the first time connecting to this system, you may be asked to accept the host key:

Click **Yes**, and the connection will be completed.



Select the run file, or run files, that you are interested in analyzing and use the translation service to convert them into the *Nexus* file format in preparation for analysis.



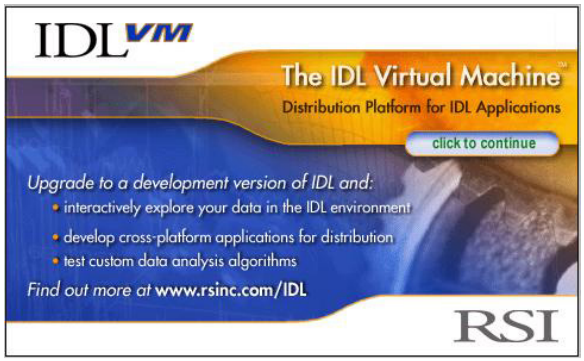
In the example shown above the runs 1314 through 1317 are being translated with the command:

TS_translate_batch 1314-1317

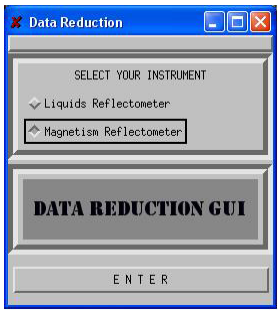
Note that the first time you run this program you will be asked one more time to type in your password.

This will create the necessary files and store them in the appropriate location so that they may be read by the *IDL* based analysis and reduction software, which is run by typing the command **data_reduction**:

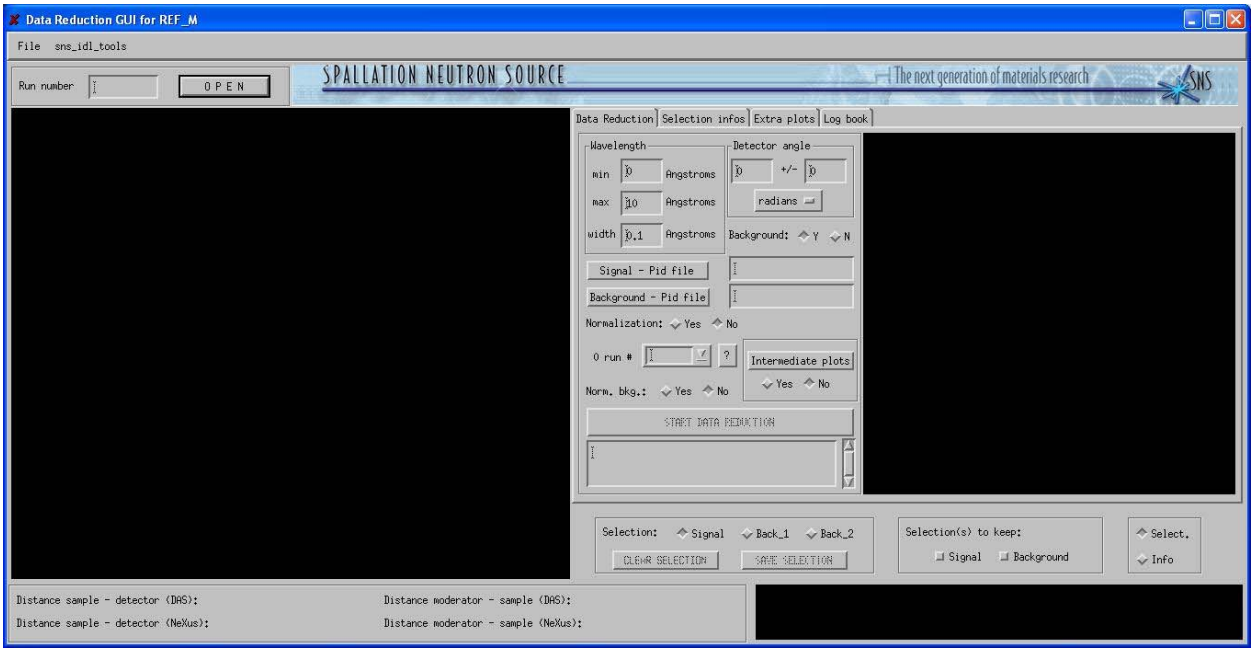
You will see the *IDL* startup widow:



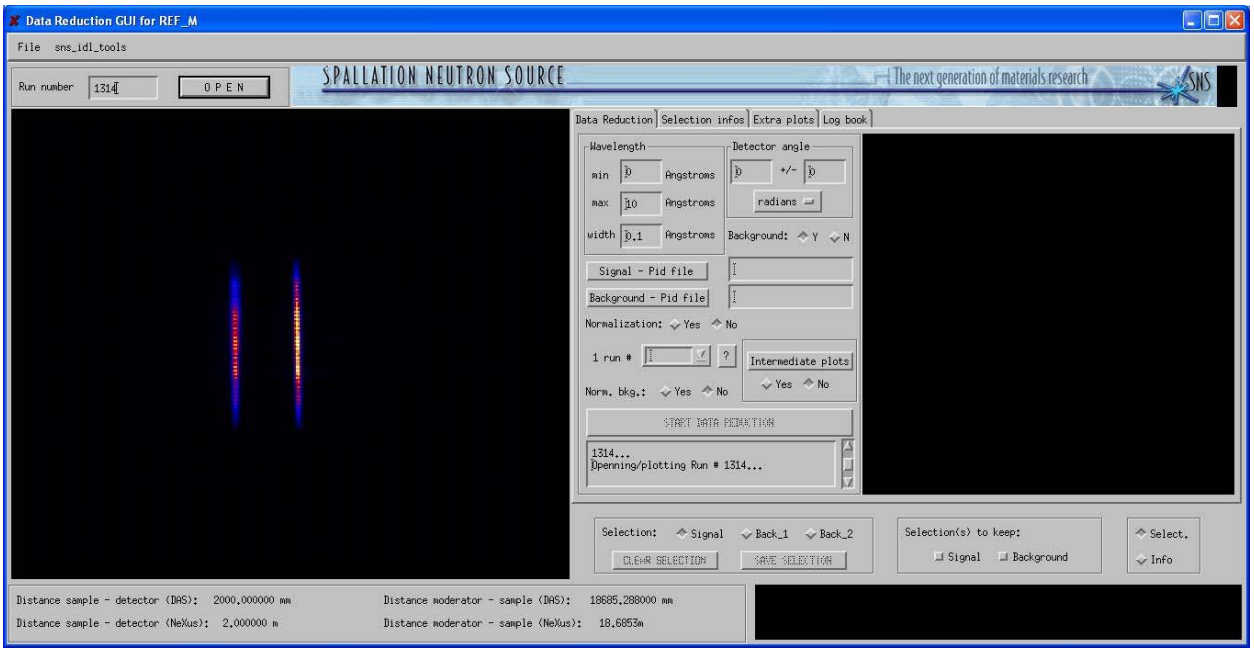
Click anywhere on the *IDL* window to continue:



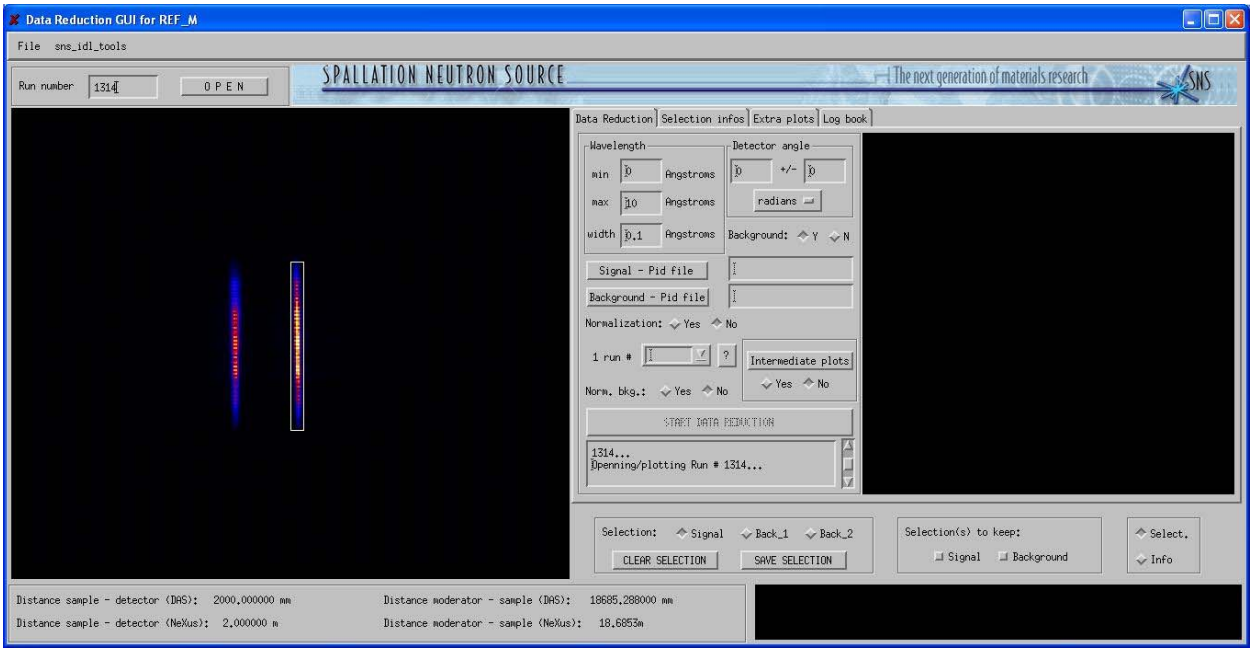
Click on the button next to **Magnetism Reflectometer** and press **ENTER** to run the **Data Reduction** GUI:



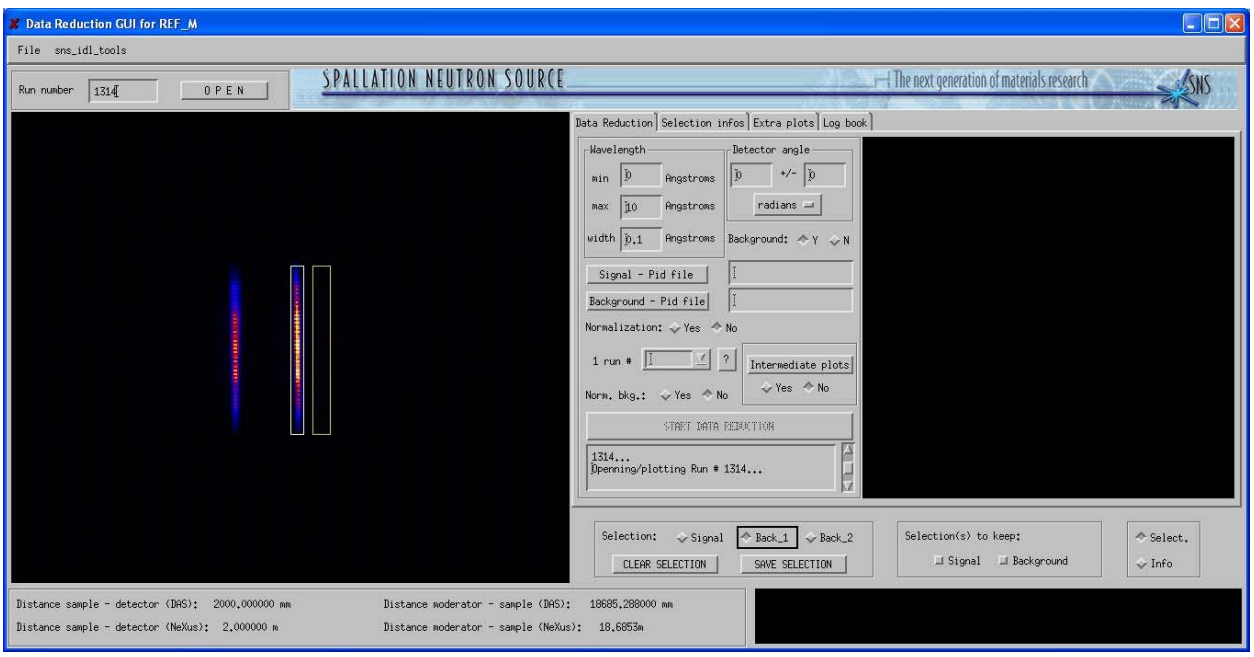
Enter the desired run number in the **Run Number** text field at the upper left hand corner of the window and press the **OPEN** button. The data file will be read, and the raw data displayed:



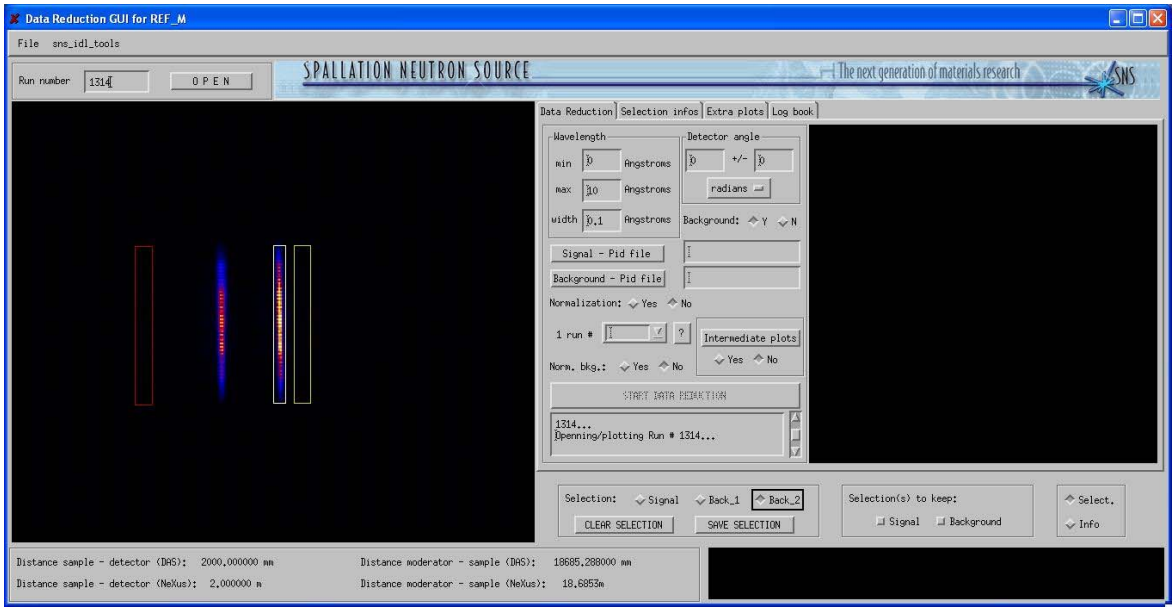
Insure that the **Signal** button on the **selection panel** is checked. Place the cursor slightly above and to the left of the desired signal region. Click and release the right mouse button. Move the cursor down and to the right until the entire signal is included within the resulting box. Click and release the right mouse button to complete your selection of the signal region.



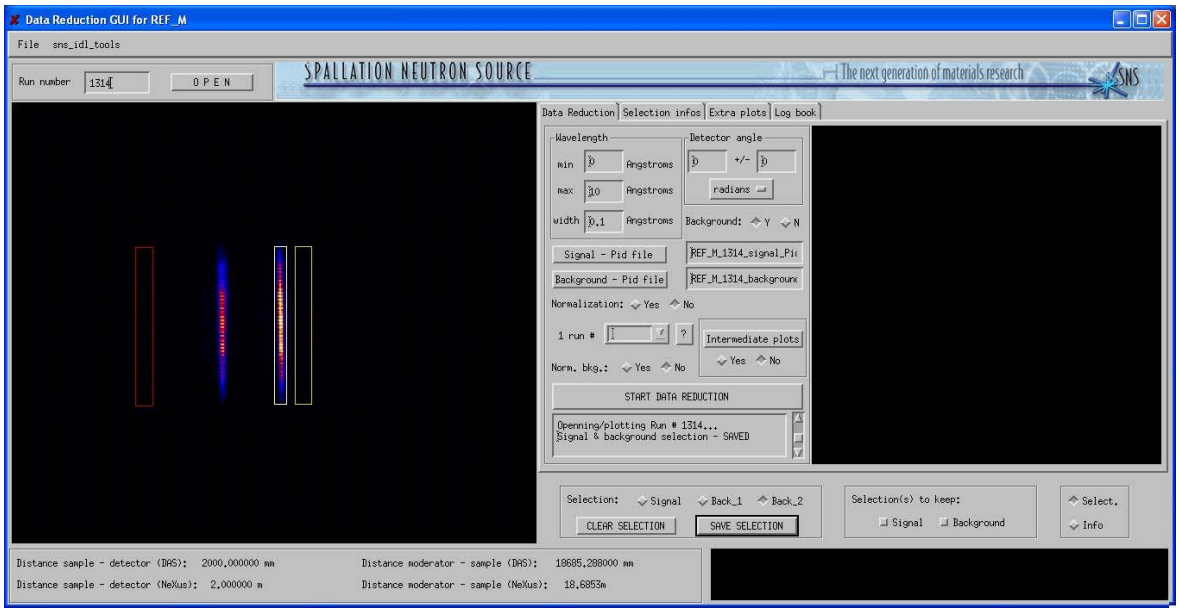
If background is to be subtracted (and it usually is) click the **Back_1** button in the **selection panel** and repeat the process used above to select a background region.



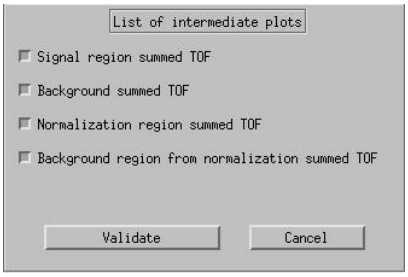
If a second background region is desired, click the **Back_2** button and repeat the process:



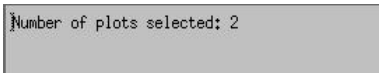
If you are satisfied with these selections, click the **SAVE SELECTION** button. Note that the message window below the **START DATA REDUCTION** button will contain the message "Signal & background selection – SAVED." If you are going to use these exact signal region and background region settings to analyze other run files you can save them to disk by clicking either or both of the buttons (**Signal** and **Background**) in the **Selection(s) to keep panel**. The signal and/or background information will be written to the same directory as the reduced data. In the example above the file names containing the stored information are **REF_M_1314_signal_Pid.txt** and **REF_M_1314_background_Pid.txt**. These files, and the information they contain, may be loaded later simply by clicking the **Signal – Pid file** button and/or the **Background – Pid file** button and selecting the desired file name.



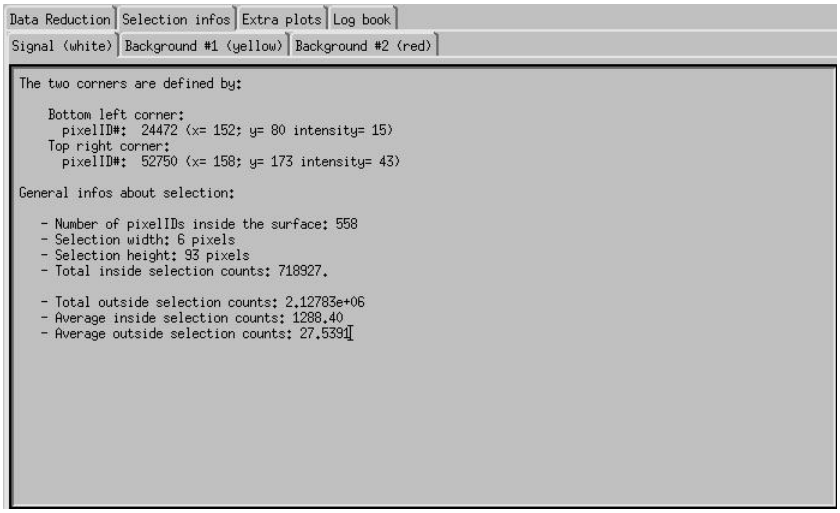
Notice that when you pressed **SAVE SELECTION** some additional information has been filled in. If you only wish to view and manipulate the intensity versus wavelength data select the **NO** button in the **Normalization section**. If you wish to normalize the data using a previously collected and reduced transmission run click the **YES** button and enter the run number of the transmission run in the **Run #** text field located next to the **Normalization Yes No** buttons. You may request to view plots of the intermediate data by clicking the **Yes** button in the **Intermediate plots** panel. You will get another window asking you to select which intermediate plots you want:



Note that by default all plots are selected. The last two plots will only be valid if you said **Yes** to **Normalization**. Adjust the selection buttons to suit your preference and click the **Validate** button. The message panel in the **Data Reduction GUI** will inform you how many valid intermediate plots will be generated:



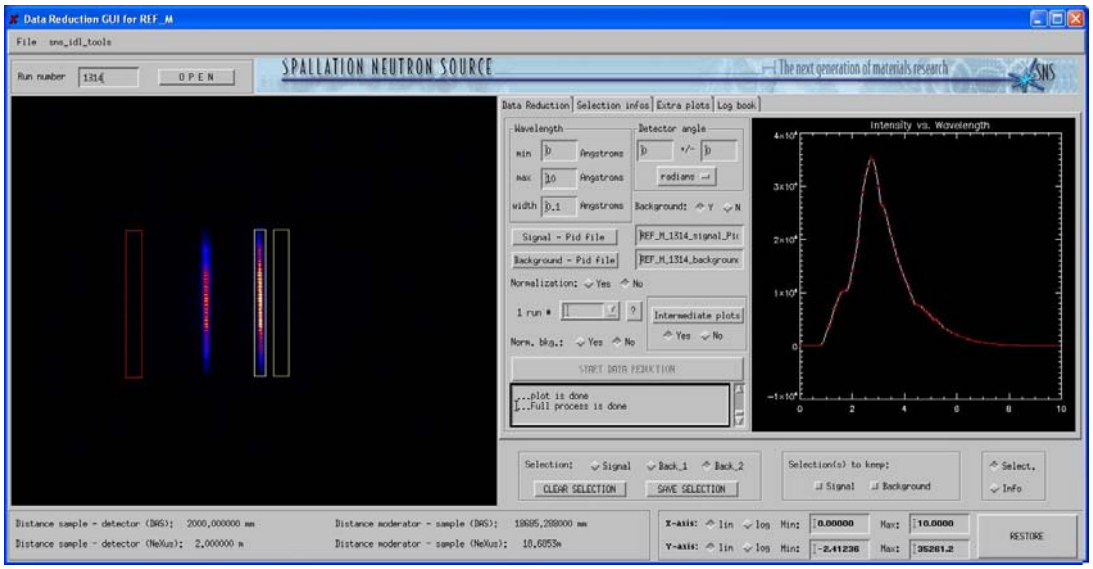
Note that since we said **No** to **Normalization** there are only two valid intermediate plots. Information on the signal and background regions that you selected using the cursor is available by clicking on the Selection info tab:



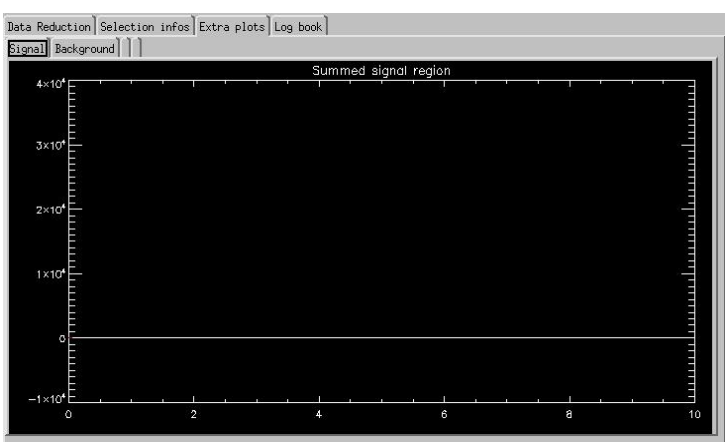
Click the tab for the region you want to view. In this example we are viewing the Signal tab, which shows that we defined our signal region to be from x channel 152 to 158 and y channel 80 to 173. Number of pixels in each direction are calculated by subtracting the high from the low

(the bounding channels are not counted towards the total number of pixels). The counts in these channels are summed, and the average counts per internal channel is calculated. Similar information is calculated for the region outside (beginning with the bounding channels) the drawn box.

The **START DATA REDUCTION** button will become active once you have completed your selection. Press the **START DATA REDUCTION** button:

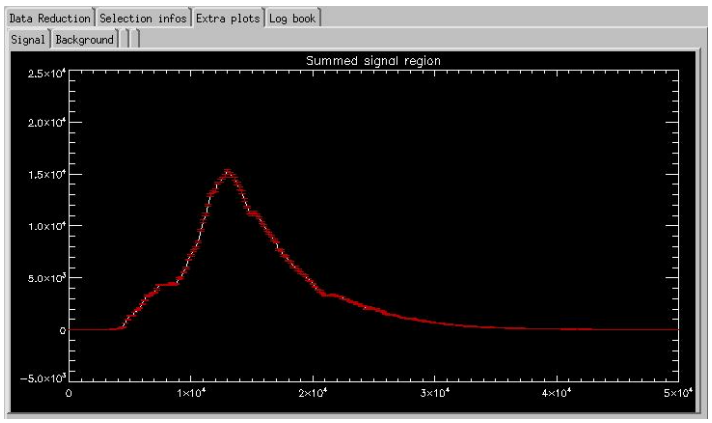


The data will be reduced, and the resulting plot will be displayed on the right hand side. Notice in this example they we did not ask for normalization, so our data plot is simply intensity versus wavelength. Also notice that the lower right hand corner now contains a panel where axes scaling can be modified, or the the default settings can be restored. You may view any requested intermediate plots by clicking on the **Extra plots** tab located in the tabs section of the GUI. Note that while the actual data is plotted as a function of wavelength on the x axis, the intermediate data is plotted as a function of time of flight on the x axis. As a result, when you simply switch tabs to the Extra plot tab to view an intermediate plot you will see nothing with the current x axis setting.

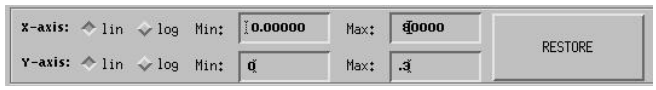


Notice that the x axis is only looking out to 10 microseconds. We will need to expand the x axis, using the x-axis Max: field in the lower left corner

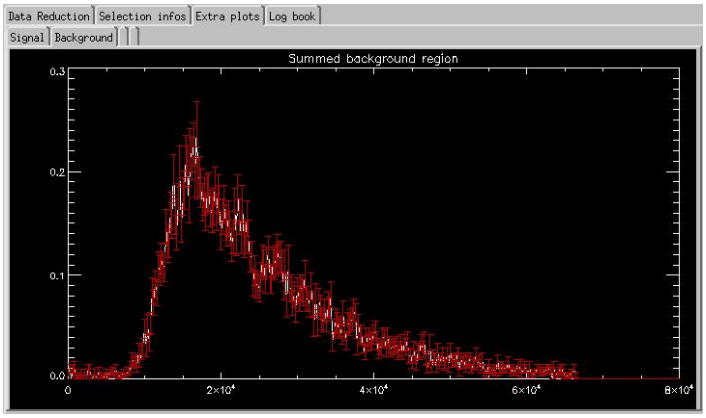
Which incorporates all the data in the plot window



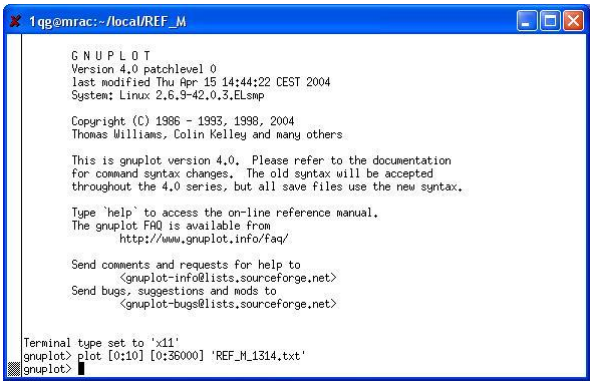
Note that the axis settings for the background are quite a bit different than those for the signal



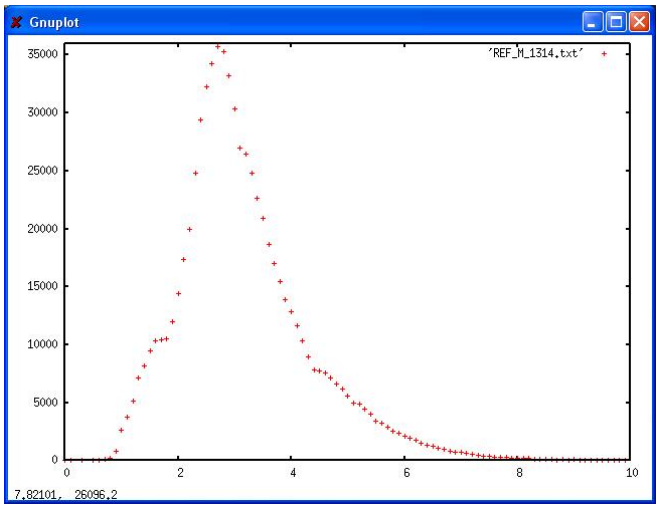
But the background region is still there:



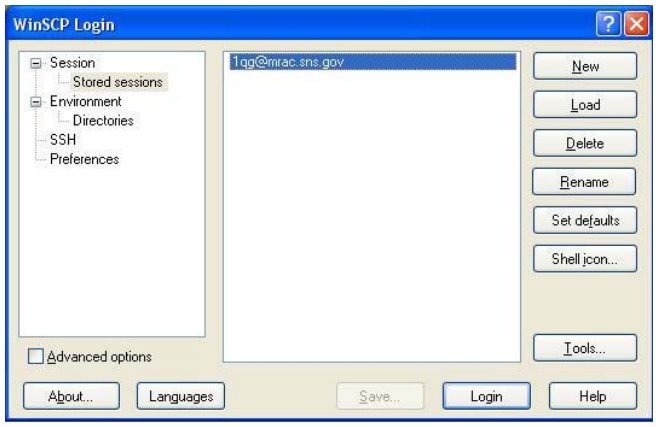
Once the *IDL* software has finished, you may use *gnuplot* to view the data; type "**gnuplot**" to start the program and get to the *gnuplot* command line. *Gnuplot* is a versatile plotting package. Obtaining a simple plot requires only the command "**plot *'filename'*** ". Note that since your data files will be in the "**local/REF_M**" subdirectory (in my case **/SNS/users/1qg/local/REF_M**) you should change your working directory to your version of that with the command "**cd ~/local/REF_M**" prior to starting *gnuplot*. You will notice that if you simply type **plot 'REF_M_1314.txt'** that the x and y axes may not be very well suited to your actual data. This is easily remedied by modifying your plot request to include x and y axis ranges. From the initial plot we notice a better x range is 0 to 10 and the y range would be 0 to 36,000. The modified plot request is now ***plot [0:10] [0:36000] 'REF_M_1314.txt'***:



This produces a more appropriate plot for your test data:

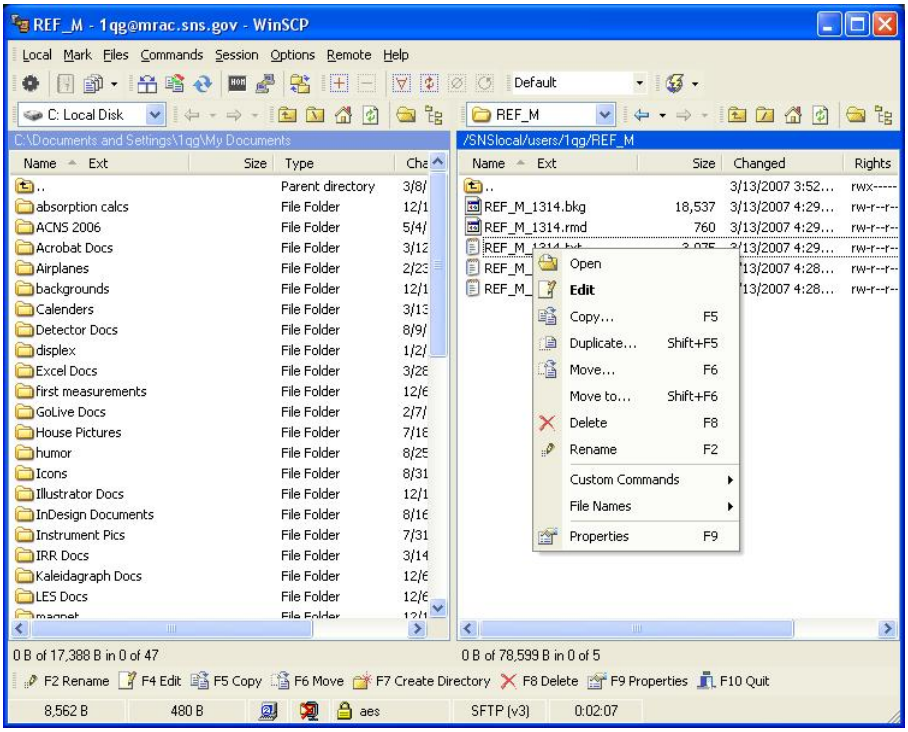


It is usually a good idea to take a quick look at your data prior to transferring it from the analysis computer to a personal computer. If you are satisfied with the file, you can use *WinSCP* (or some other secure copying package) to transfer it to your computer. You will need to define a session for mrac.sns.gov:



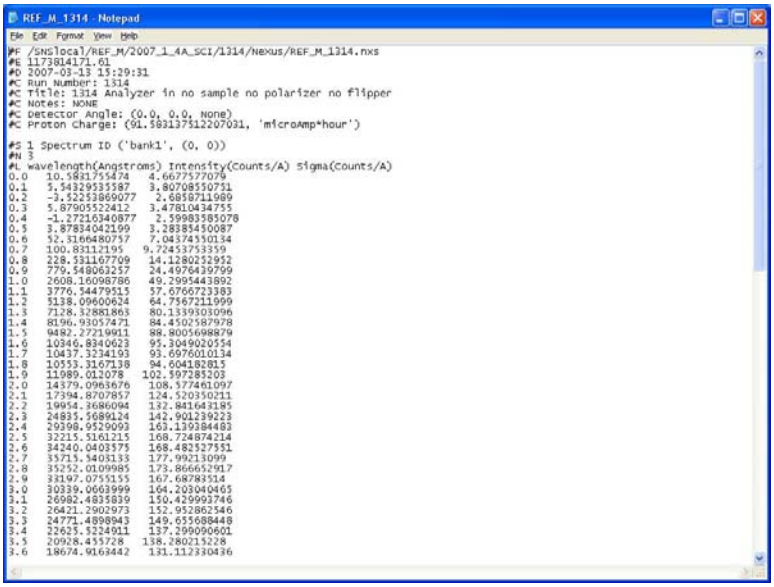
Click Login and you will be prompted for your **XCAMS** password:

Once you have the connection established, change to the directory containing the data files and select the desired file. Right click on the desired file and select **Copy**:



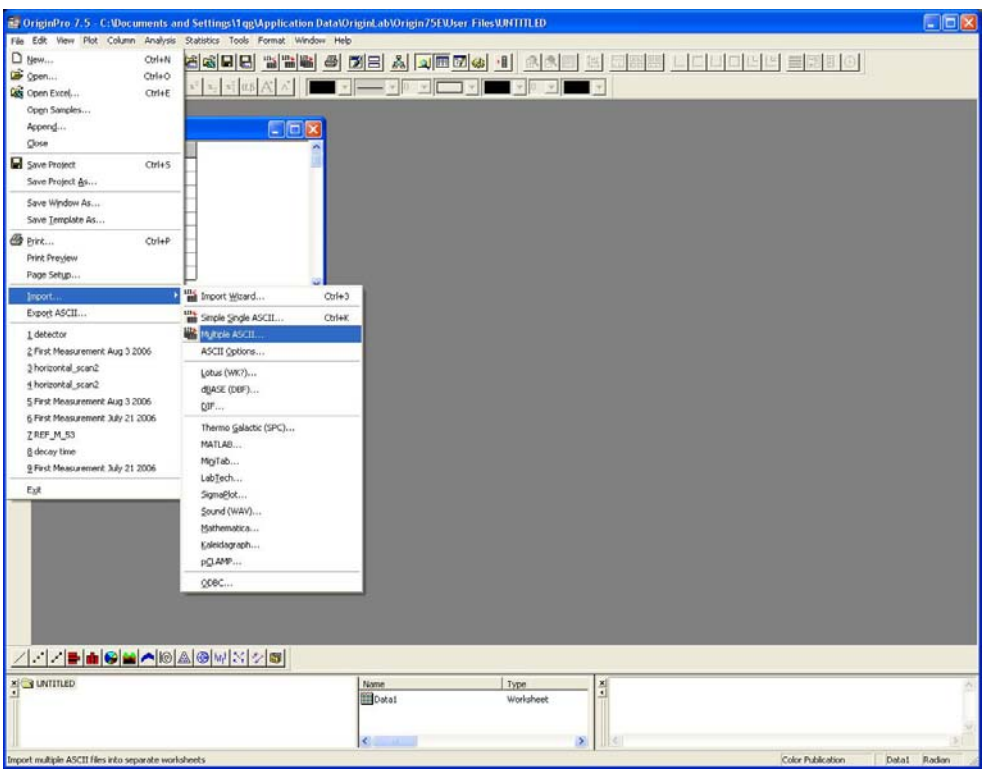
Pick the destination for the data file:

The data file may now be viewed or manipulated on your PC:



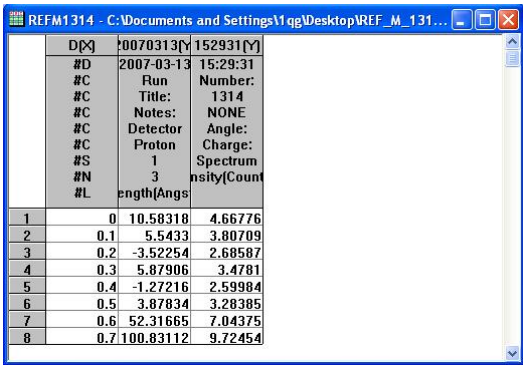
```
REF_M_1314 - Notepad
File Edit Format View Help
#F /SNSlocal/REF_M/2007_1_4A_SCI/1314/Nexus/REF_M_1314.nxs
#E 1173814171.61
#D 2007-03-13 15:29:31
#C Run Number: 1314
#C Title: 1314 Analyzer in no sample no polarizer no flipper
#C Notes: NONE
#C Detector Angle: (0.0, 0.0, None)
#C Proton Charge: (91.583137512207031, 'microAmp*hour')

#S 1 Spectrum ID ('bank1', (0, 0))
#N 3
#L wavelength(Angstroms) Intensity(Counts/A) sigma(Counts/A)
0.0   10.5821755474   4.6677577079
0.1   5.54329535587   3.80708550751
0.2   -3.52253869077   2.6858711989
0.3   5.87905522412   3.47810434755
0.4   -1.27216340877   2.59983585078
0.5   3.87834042199   3.28385450087
0.6   52.3166480757   7.04374550134
0.7   100.83112195   9.72453753359
0.8   228.531167709   14.1280252952
0.9   779.548063257   24.4976439799
1.0   2608.16098786   49.2995443892
1.1   3776.54479515   57.6766723383
1.2   5138.09600624   64.7567211999
1.3   7128.32881863   80.1339303096
1.4   8196.93057471   84.4502587978
1.5   9482.2721991   88.8005698879
1.6   10346.8340623   95.3049020554
1.7   10437.3234193   93.6976010134
1.8   10553.3167138   94.604182815
1.9   11989.012078   102.597285203
2.0   14379.0963676   108.577461097
2.1   17394.8707857   124.520350211
2.2   19954.3686094   132.841643185
2.3   24833.5689124   142.901239223
2.4   29398.9529093   163.139384483
2.5   32215.5161215   168.724874214
2.6   34240.0403575   168.482527551
2.7   35715.5403133   177.99213099
2.8   35252.0109985   173.866652917
2.9   33197.0755155   167.68783514
3.0   30339.0663999   164.203040465
3.1   26982.4835839   150.429993746
3.2   26421.2902973   152.952862546
3.3   24771.4898943   149.655688448
3.4   22625.5224911   137.299090601
3.5   20928.455728   138.280215228
3.6   18674.9163442   131.112330436
```

All the lines beginning with the "#" symbol are comment lines containing information about conditions under which the file was collected. Using *Origin*, or another software package, you can plot, manipulate and fit your data file. Starting *Origin*, select **Import, Multiple ASCII** from the **File** menu:



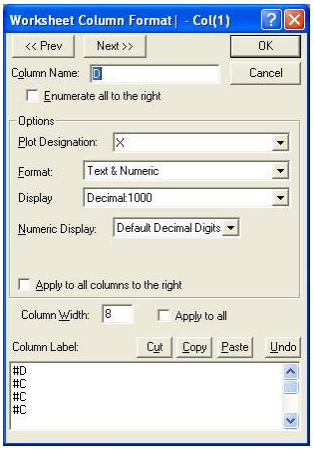
Select the desired file name:

Origin will read the comment lines and generate column labels that are not really appropriate for the data.

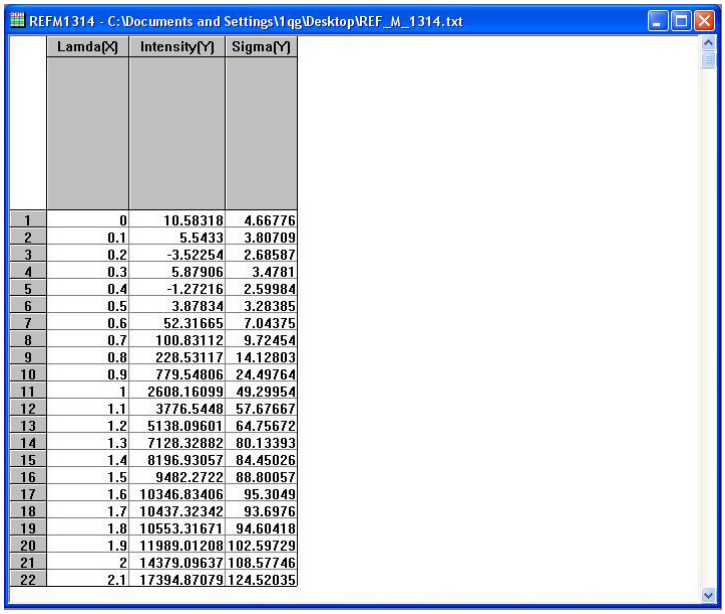


	D(X)	20070313(Y	152931(Y)
	#D	2007-03-13	15:29:31
	#C	Run	Number:
	#C	Title:	1314
	#C	Notes:	NONE
	#C	Detector	Angle:
	#C	Proton	Charge:
	#S	1	Spectrum
	#N	3	nsity(Count
	#L	ength(Angs	
1	0	10.58318	4.66776
2	0.1	5.5433	3.80709
3	0.2	-3.52254	2.68587
4	0.3	5.87906	3.4781
5	0.4	-1.27216	2.59984
6	0.5	3.87834	3.28385
7	0.6	52.31665	7.04375
8	0.7	100.83112	9.72454

These labels may be changed to something more appropriate simply by double clicking on them:



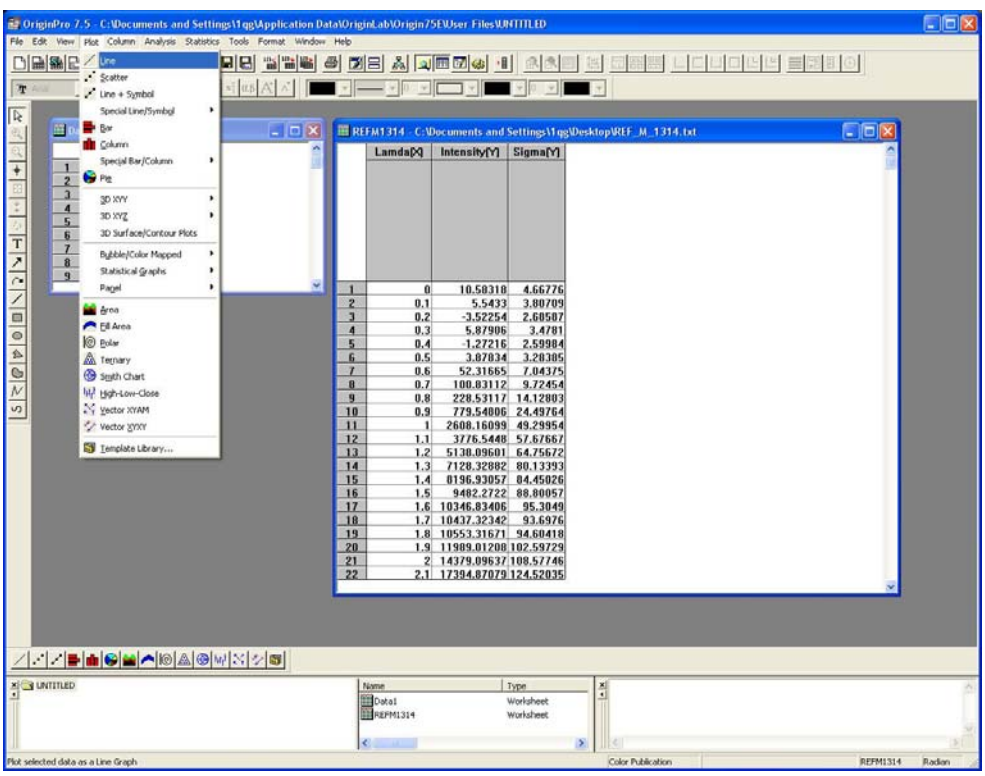
Change the column name, and remove all the contents of the **Column Label** field at the bottom. Repeat this process for all labels until you get labels you like.



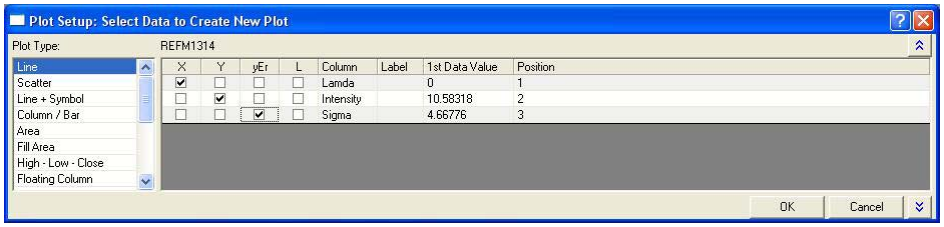
REFM1314 - C:\Documents and Settings\1qg\Desktop\REF_M_1314.txt

	Lamda[X]	Intensity[Y]	Sigma[Y]
1	0	10.58318	4.66776
2	0.1	5.5433	3.80709
3	0.2	-3.52254	2.68587
4	0.3	5.87906	3.4781
5	0.4	-1.27216	2.59984
6	0.5	3.87834	3.28385
7	0.6	52.31665	7.04375
8	0.7	100.83112	9.72454
9	0.8	228.53117	14.12803
10	0.9	779.54806	24.49764
11	1	2608.16099	49.29954
12	1.1	3776.5448	57.67667
13	1.2	5138.09601	64.75672
14	1.3	7128.32882	80.13393
15	1.4	8196.93057	84.45026
16	1.5	9482.2722	88.80057
17	1.6	10346.83406	95.3049
18	1.7	10437.32342	93.6976
19	1.8	10553.31671	94.60418
20	1.9	11989.01208	102.59729
21	2	14379.09637	108.57746
22	2.1	17394.87079	124.52035

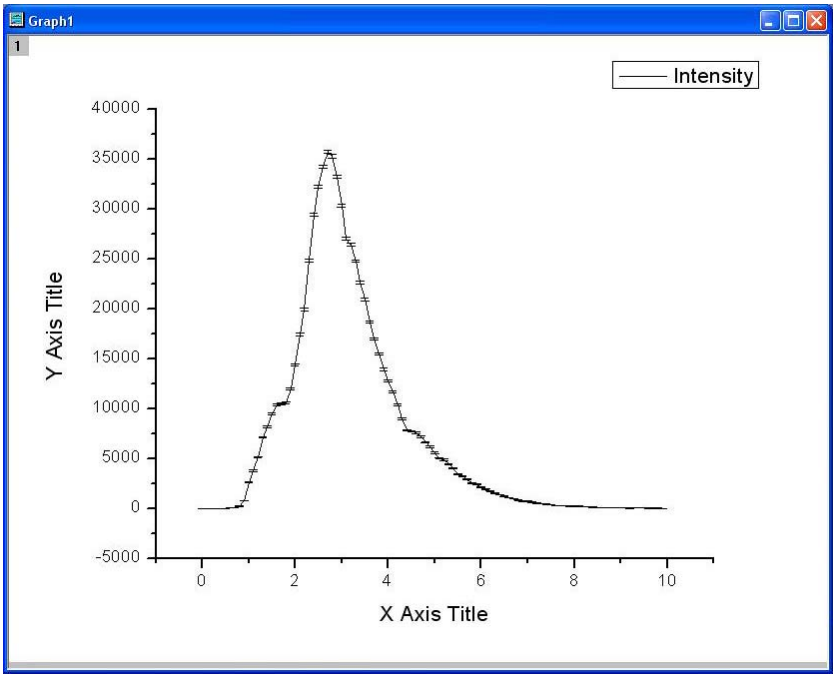
The data may now be plotted by selecting the desired plot type from the **Plot** menu:



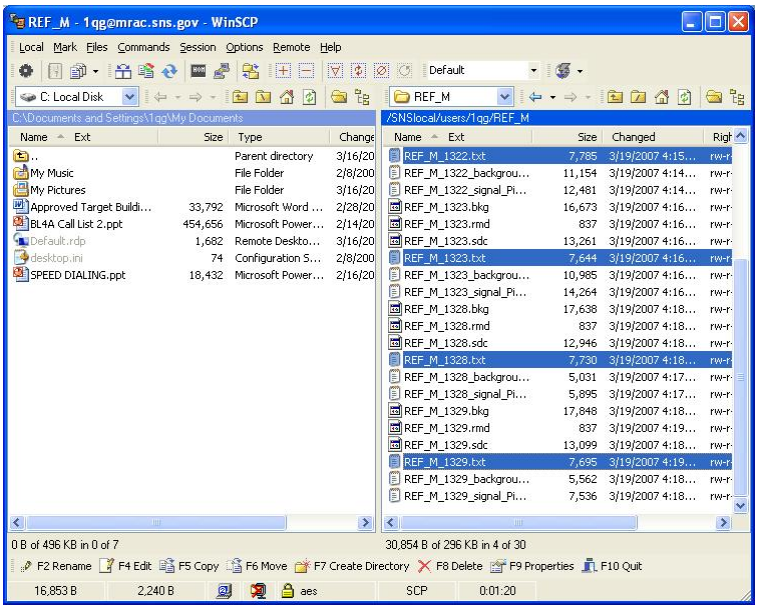
And selecting the axes:



The data will now be plotted:



Note that this plot looks very similar to the one we generated with *gnuplot*. The benefit of using *Origin* is demonstrated more clearly in the following example: generating reflectivity data. While the *IDL* based data reduction software is capable of creating reflectivity curves, there may be times when you want to generate the reflectivity data from the raw data by hand. For this example we are going to need four run files: two with only the transmitted beam at different collimations, and two of the beam reflected off our sample (in this case 500 Å of iron on a silicon substrate) These run files were reduced in the manner described above and will be copied to my local PC by selecting each file in *WinSCP* while holding down the **Ctrl** key.



Now that I have them, I am going to rename **REF_M_1322** and **REF_M_1323** to **TRANS_M_1322** and **TRANS_M_1323**, so I call tell the transmitted files from the reflected files. So now we have four files on the desktop:

TRANS_M_1322.TXT	.6 mm collimation transmission run
TRANS_M_1323.TXT	1.2 mm collimation transmission run
REF_M_1328.TXT	0.28 degree data run
REF_M_1329.TXT	0.62 degree data run

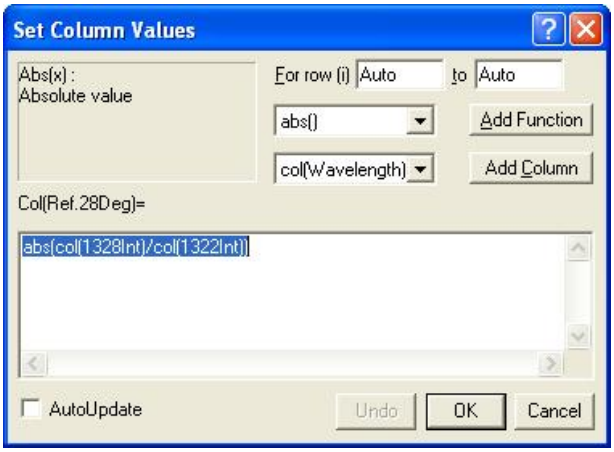
It's a good ides to give these files a more descriptive name so that later when you have a whole bunch of files you can tell them apart. Since the data in these files is from a 500 Å Iron (Fe) sample on a silicon substrate the data files could be named **FE1228.TXT** and **FE1329.TXT**

I started *Origin*, and opened a new data file. Since all the collected data (transmission and reflection) was collected with the same time binning the first column of each file (the wavelength column) is the same. So I only include one column of wavelength data from any of the files, and copy the last two columns from each of the four files. This gives me one data file with nine columns of data, for which I used column labels that I could interpret. I also included six empty columns that will be used to store the calculated reflectivity and uncertainty for each of the two collected angles, as well as the calculated value of **q** ($q=4\pi SIN\theta/\lambda$) for those angles. That is a total of fifteen columns of data:

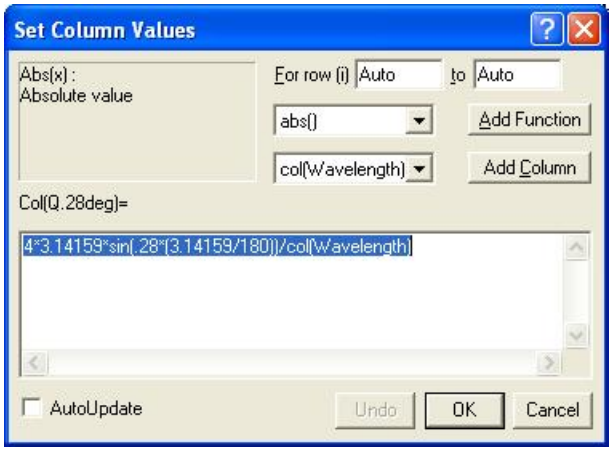
Data1

	Wavelength[X]	1322Int[Y]	1322Sigma[Y]	1323Int[Y]	1323Sigma[Y]	1328Int[Y]	1328Sigma[Y]	1329Int[Y]	1329Sigma[Y]
1	0	16.47087	4.13909	13.67755	4.00853	34.06486	5.92185	-1.09904	1.01772
2	0.05	3.10925	1.75431	0.63015	1.15893	1.46199	1.26712	-5.81714	0.82538
3	0.1	2.32293	1.34594	1.62729	0.93952	0.08537	0.90373	-2.0797	0.9422
4	0.15	1.59455	1.2106	1.92905	1.29423	-1.79925	0.0517	0.68208	1.07383
5	0.2	0.25999	0.39152	1.11694	0.9852	-3.2824	0.08471	-4.38455	0.2922
6	0.25	0.19398	1.01136	0.95004	1.42052	-1.32944	0.10059	0.43884	1.00006
7	0.3	2.46364	1.58509	1.71215	1.02432	1.15472	0.98936	-1.41386	0.04883
8	0.35	-1.75297	0.44805	1.65347	1.27201	0.12806	1.13159	0.0137	0.63254
9	0.4	-1.87299	0.55498	-0.68125	0.02112	0.59236	1.04648	1.73433	1.00313
10	0.45	1.98003	1.61651	0	0	0.66607	0.96577	1.82942	1.44904
11	0.5	-0.48478	0.38543	0	0	0.87297	1.41266	1.13965	1.43841
12	0.55	7.28785	2.22555	17.95861	3.49013	-1.29124	0.17903	0.57481	1.42542
13	0.6	48.20909	5.53299	66.20947	6.30009	-1.02775	0.9036	-1.2272	0.90343
14	0.65	86.91421	7.2197	131.33239	8.79447	-0.69946	0.84079	0.82963	1.12722
15	0.7	128.80823	9.05147	204.11065	11.42704	-0.56069	0.46999	2.98127	1.47681
16	0.75	189.88779	12.17122	301.3931	15.3548	-0.08768	0.89423	-0.20566	0.50066
17	0.8	223.71467	13.89616	391.77097	18.46916	0.90847	1.00574	0.69517	1.00003
18	0.85	293.65437	14.24468	469.46333	18.543	-1.06717	0.36391	-2.26832	0.26361
19	0.9	568.04452	18.45768	813.48976	21.89476	-0.18914	1.14217	-0.75438	0.86468
20	0.95	1463.85974	29.7419	1916.87862	33.96511	1.79317	1.20781	1.67734	1.3562
21	1	3204.38568	47.60694	3940.71632	52.77981	1.15139	0.66475	-0.37345	0.76976
22	1.05	3488.1174	54.00755	4464.89651	61.34286	-0.09601	0.97921	-0.4861	0.01471
23	1.1	4309.49783	61.74358	5206.3614	67.89065	-0.00218	0.02221	1.5888	1.42315
24	1.15	4003.56567	52.27381	4804.96483	57.13435	0.33944	0.33944	-1.97546	1.02944
25	1.2	4739.36363	53.0398	5841.86249	58.85255	1.18081	0.84083	-0.32581	1.25832
26	1.25	5955.88449	60.93965	7305.84858	67.43987	1.88187	1.10143	0.59464	1.30657
27	1.3	8273.84099	79.62807	9554.18949	85.19083	2.27503	1.58557	0.36482	1.02375
28	1.35	9611.77534	91.86448	10964.48827	98.13772	4.47539	2.01435	5.09274	2.45688
29	1.4	8237.80131	79.58979	9278.00601	84.57758	5.45373	1.98224	4.00735	2.12415
30	1.45	9872.5926	79.10766	10950.19559	83.34588	8.18235	2.37222	-1.76969	1.22929
31	1.5	8599.98126	71.13396	9817.84407	76.0362	8.69831	2.50624	1.6723	1.18154
32	1.55	7773.89781	71.99278	9629.05021	80.38409	8.39027	2.75425	-1.40255	1.24648
33	1.6	8866.04405	86.4236	11848.49746	100.31305	12.06955	3.27705	2.69738	2.57712
34	1.65	10812.92061	94.78978	15617.91777	113.86602	16.79638	4.05628	5.04478	2.67687
35	1.7	15452.47956	103.49446	22983.47964	125.69147	29.13487	4.4401	3.20212	2.48475
36	1.75	15440.38839	97.08146	23694.09642	120.30714	47.19011	5.68258	4.83927	2.61781
37	1.8	14673.45669	94.91573	23107.65643	119.33631	68.1331	6.78716	3.18334	2.63443

Keep in mind that *Origin* accepts angles in radians, so you have to convert the sample angle from degrees to radians (by multiplying by $\pi/180$). To calculate the reflectivity data, select the column you want to fill in with the reflectivity data and select **Set Column Values** from the **Column** menu:

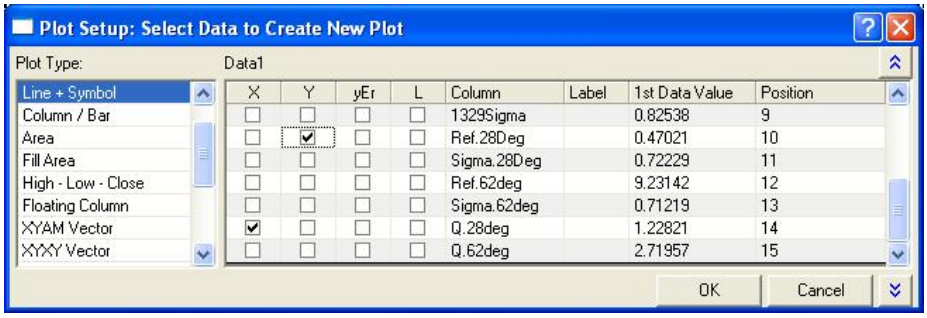


Note the column label where the data is to be stored (Ref.28Deg), and the calculation (abs(col(1328Int)/col(1322Int)). This is dividing the reflected data at .28 degrees by the transmitted data with a .6 mm collimation and storing the absolute value of the result in the column labeled Ref.28Deg. Repeat the process for the .62 degree reflected data and the 1.2 mm collimated transmission data, and store the result in the column labeled Ref.62Deg. In a similar fashion we calculate the q columns (Q.28Deg and Q.62Deg):

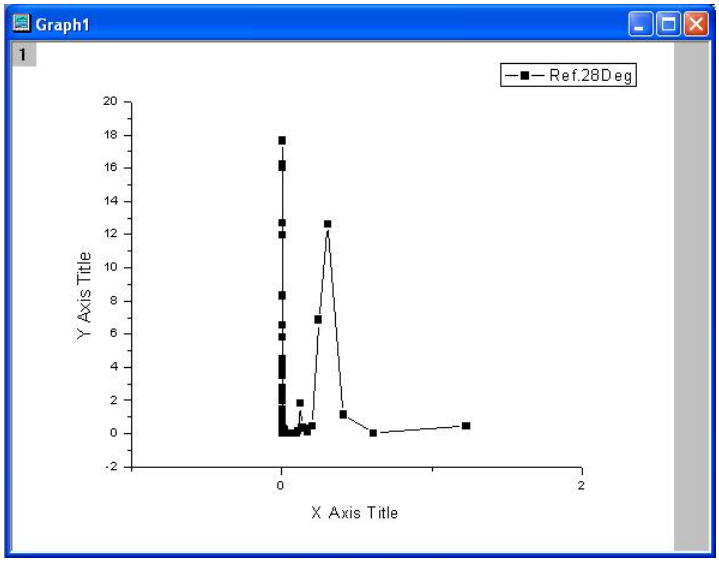


Again, note the column label (in this example Q.28Deg), and the calculation (4*3.14159*sin(.28*(3.14159/180))/col(Wavelength) for the .28 degree data). We should now have all the data necessary to generate **reflectivity versus q** plots for both the sample angles we collected. Now select **Line + Symbol** from the **Plot** menu:

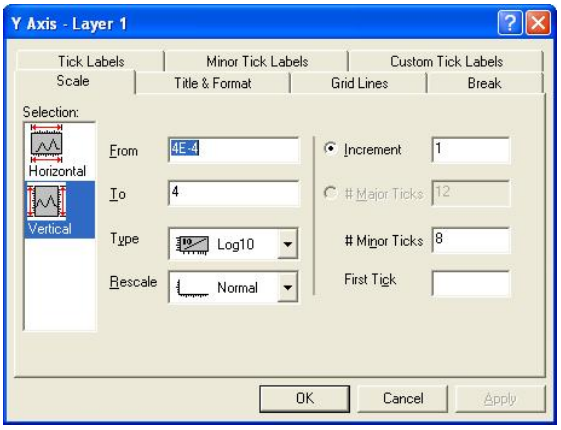
You will get the **Plot Setup** window:



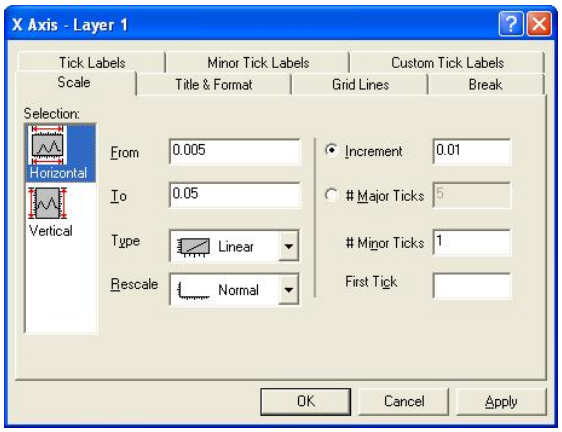
Select the appropriate **q** and reflectivity data to plot. Your initial plot results will probably not look quite right:



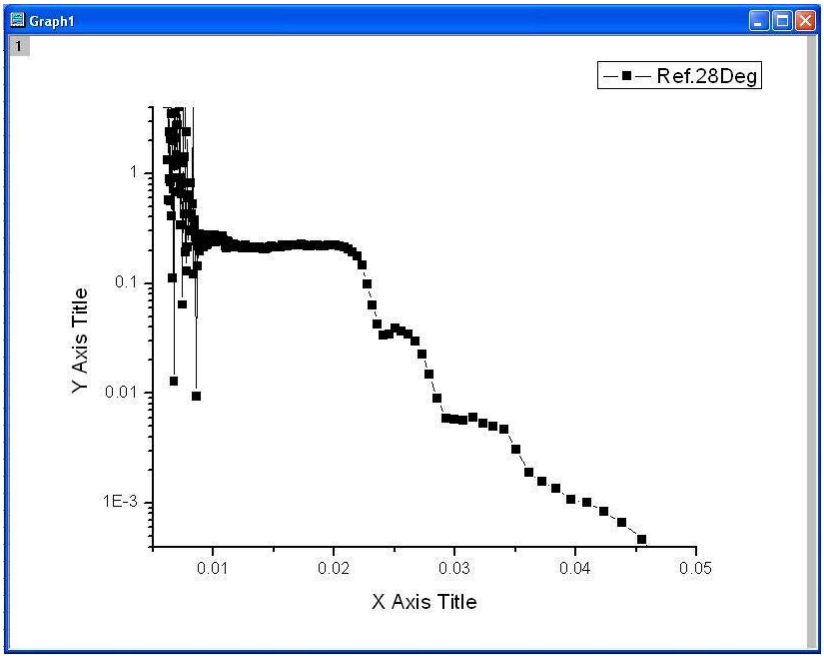
Double click on the **Y axis** (the axis, not the label):



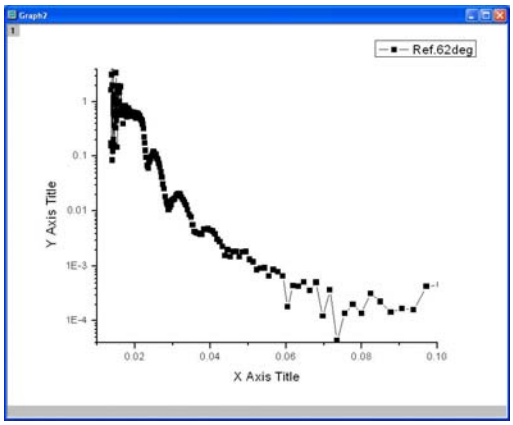
Change the **Type** to **Log10**; change **From** to **0.0004**, and **To** to **4** and click **Apply**. Click on the **Horizontal** button to switch to the X-axis:



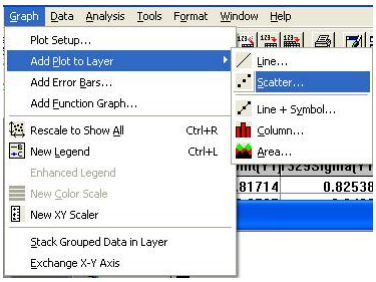
Change **From** to **0.005**, and **To** to **0.05** and click **OK**. You will now have a more recognizable reflectivity plot:



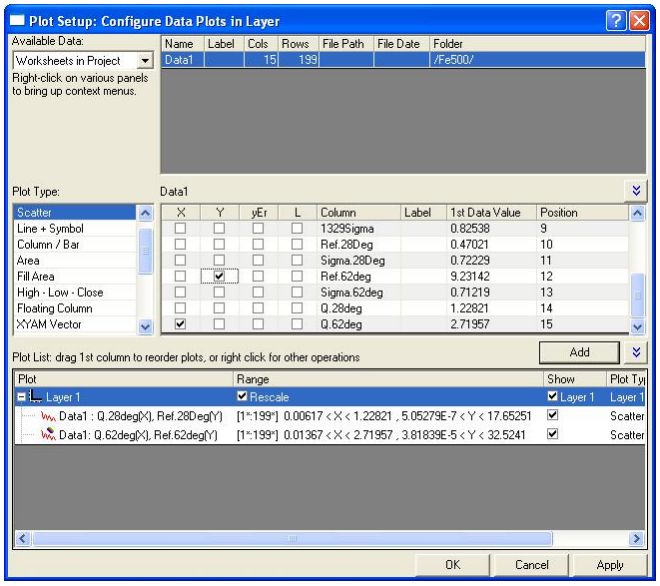
A similar plot can be generated for the higher angle data:



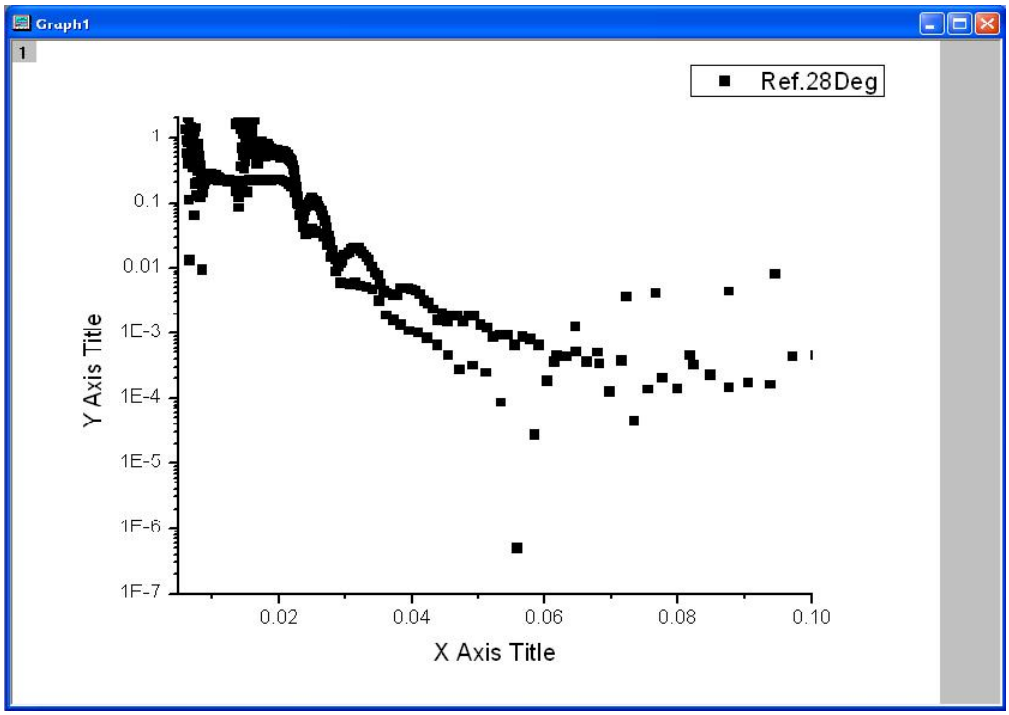
We can put these two plots together if we want. Start with the .28 degree plot, and select **Add Plot to Layer – Scatter** from the **Graph** menu



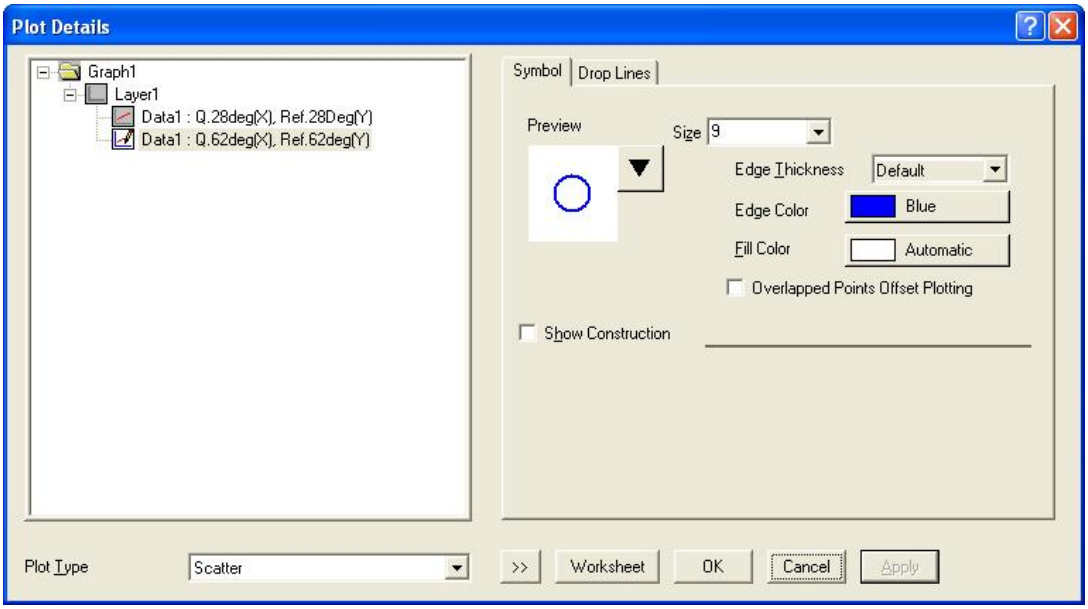
Select the 0.62 degree data (Q.62 Deg for x and Ref.62deg for y) and click **Add**:



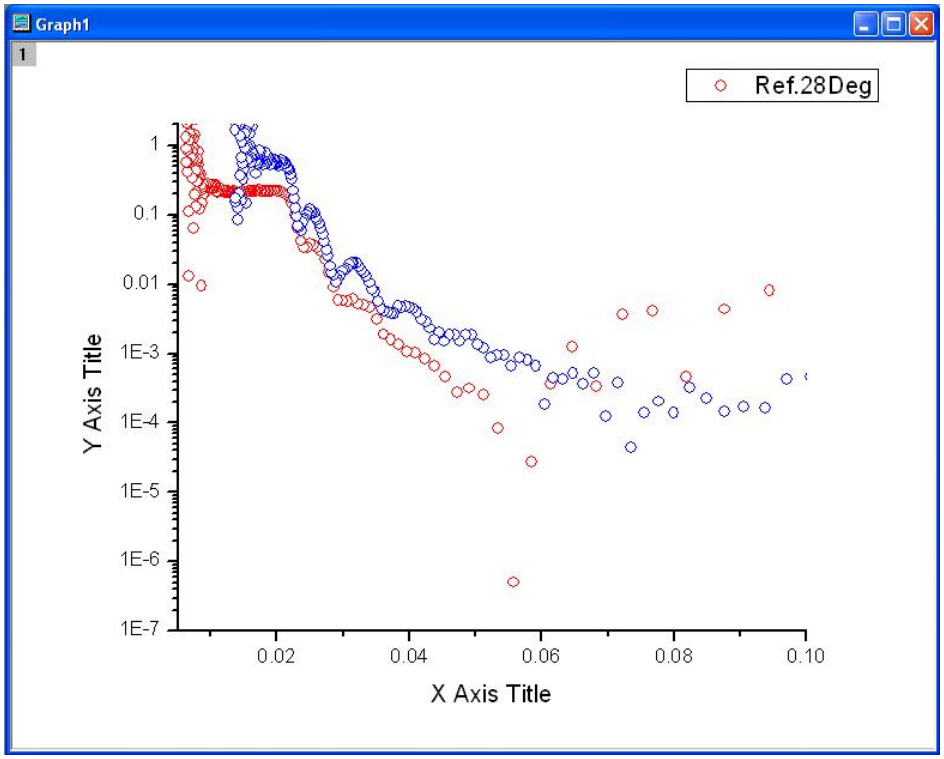
Once you click **Add** you will see the .62 degree data listed in the bottom of the window. Click **Apply** and then **OK**. You will have to adjust the axes again, but both plots will be visible:



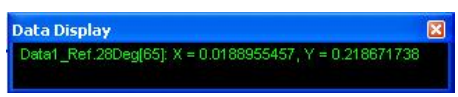
Click on the legend in the plot and change the symbol and color of the two plots:



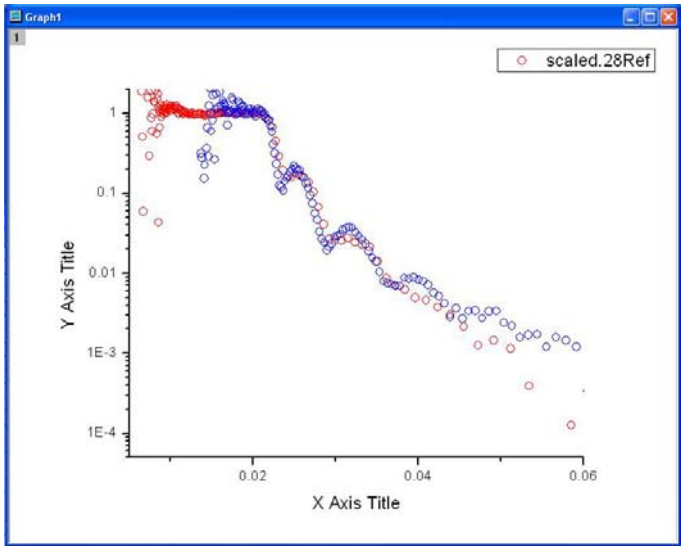
I like to keep the symbol the same but change the color…your choices may be different:



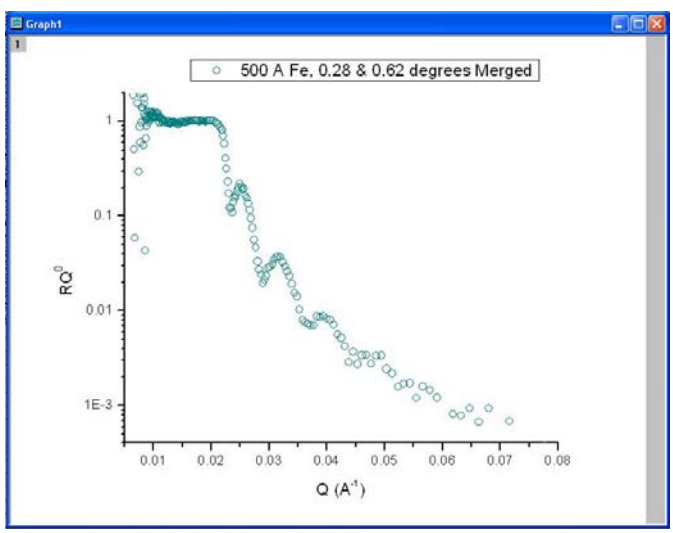
Notice that the regions of total reflection which should, by definition, equal 1, need to be scaled. Use the data reader tool (the tool)and click somewhere along the flat section of the total reflection plateau to read the reflectivity value. A window will appear displaying the x and y axis values for the point you chose.

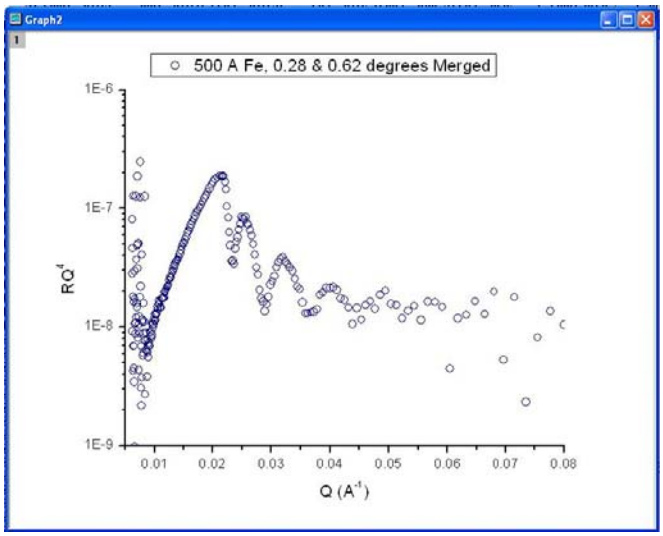


It is the y value that corresponds to the reflectivity, and which needs to be scaled to 1.0. Determine the scaling factor to adjust this value to 1.0 and then apply it to all the reflectivity in that data set. In our .28 degree example the value is 0.2186717, which requires a scaling factor of 4.5730654. A similar scaling factor can be determined for the 0.62 degree data. Now add two new columns. Into one add the .028 degree reflectivity data multiplied by the 0.28 scaling factor, and repeat the process for the 0.62 degree data and the 0.62 degree scaling factor. Now duplicate the plotting process for the scaled data:



Now the total reflection plateau for each data set is at 1, which is what it should be. Notice we now have some agreement of features between the two plots, which we should also have. However we also notice that there is too much overlap between these two angles, which tells us that we picked angles that are too close together. Normally only a small overlap in the **q** range is required to splice two reflectivity curves together; something on the order of 0.02 in **q** range should be sufficient. We can merge the two files in a simple way, by hand, by cutting and pasting in q ranges and the associated reflectivity data, from the two runs. I chose the q value to splice my data to be q = .02158 which has pretty good agreement between the two curves, and occurs right about at the critical edge:



Now we see the total reflection plateau from the 0.28 degree run and the higher q data, starting at about the critical edge, from the 0.62 degree run. Notice that there is no distinguishable splice at

the interface, which means that we chose a good point for the splice. We can add a final column and generate the merged RQ^4 –vs- Q plot: