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FOCUS DATA REDUCTION

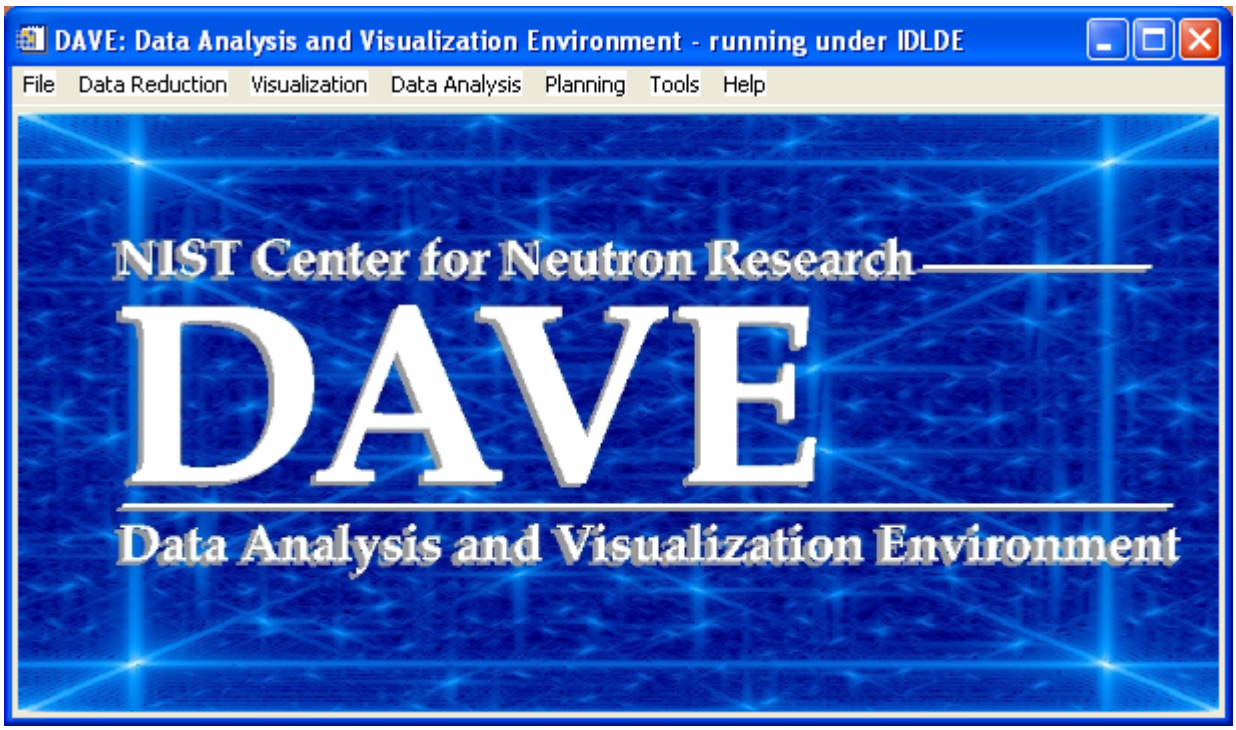
Contents:

1. Introduction

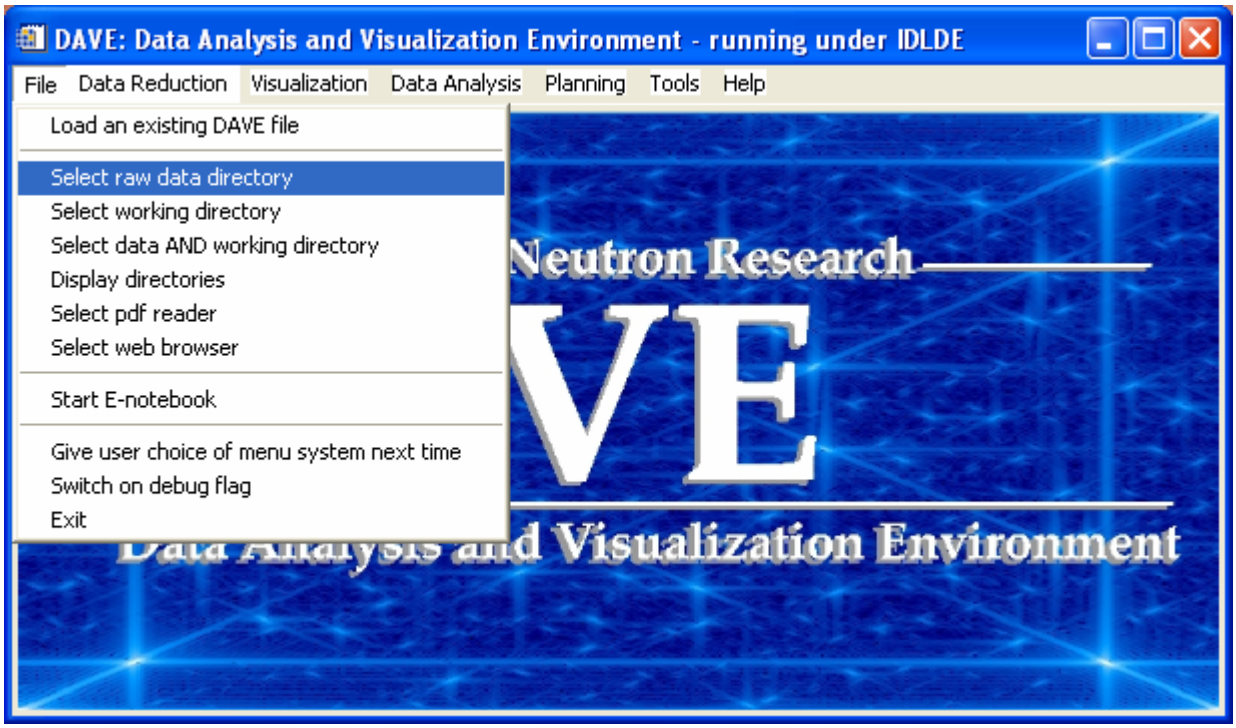
This document describes the program to reduce data collected on the direct time-of flight spectrometer FOCUS, at the SINQ facility located at the Paul Scherrer Institut in Switzerland. The program is known as FDR, which stands for Focus Data Reduction and should be easy to remember by those famililar with American history. FDR was written in IDL 6.1/6.2. and is incorporated within the DAVE program package. DAVE stands for "Data Analysis and Visualisation Environment", and is essentially a series of programs developed by Rob Dimeo and his colleagues at the NIST facility, Washington D.C., for the reduction and analysis of inelastic neutron scattering data. Once the user has reduced a raw FOCUS file, the data analysis programs within the DAVE package will be at his disposal.

2. The Basic Program Interface

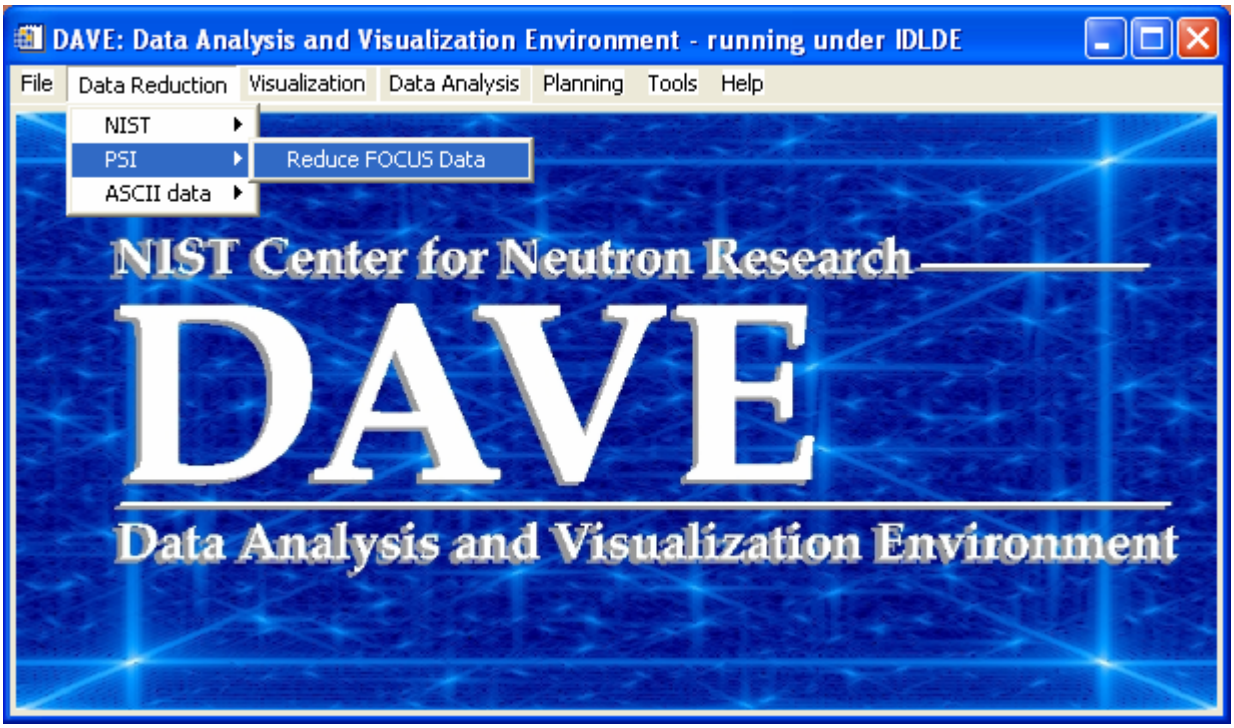
When DAVE is launched in classic view, the user should see a screen like the one shown below:



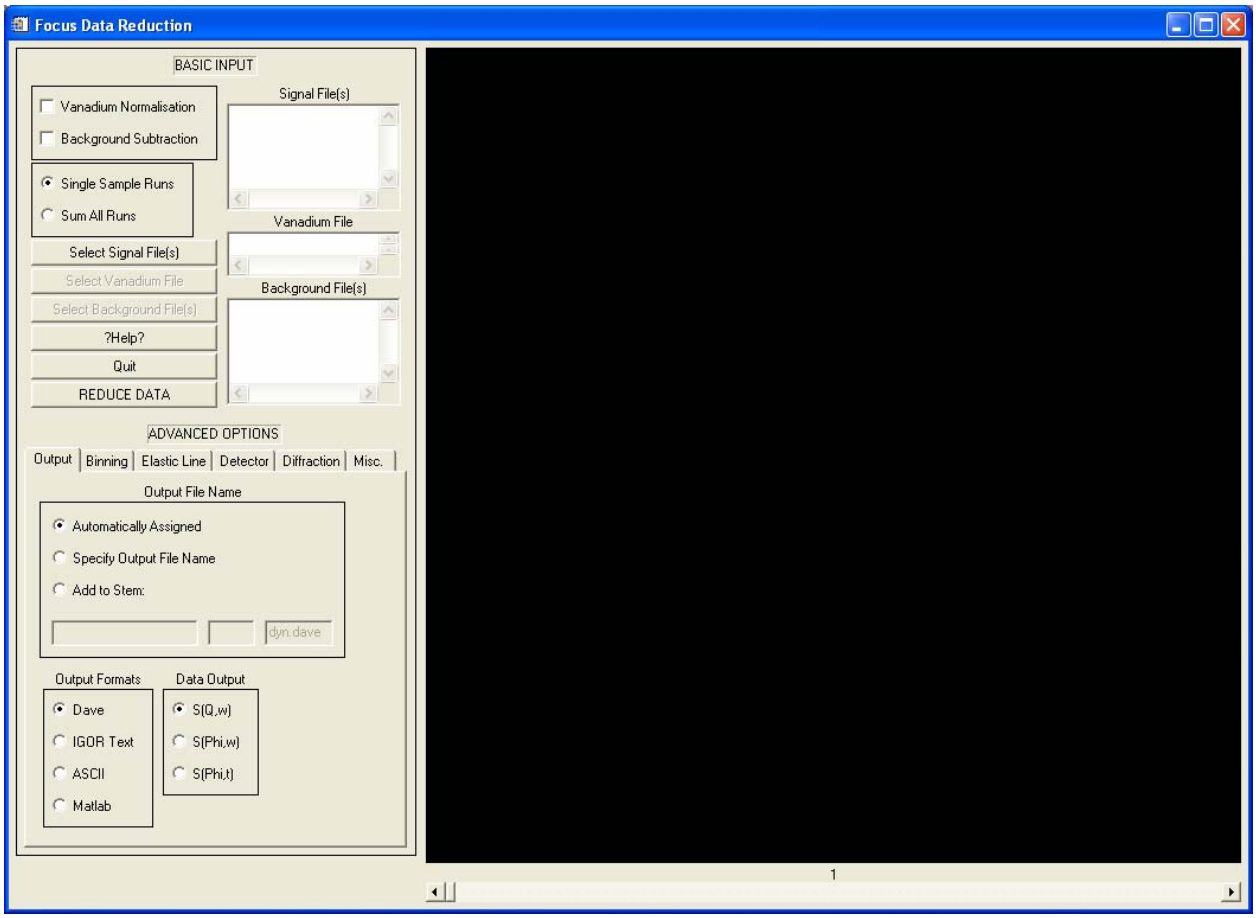
First of all, the program environment needs to be configured, if this has not been done already. This is achieved by clicking on the "File" menu header and selecting the options appropriately. The raw data files should be contained in the raw data directory. All the files that the program outputs will be saved to the working directory.



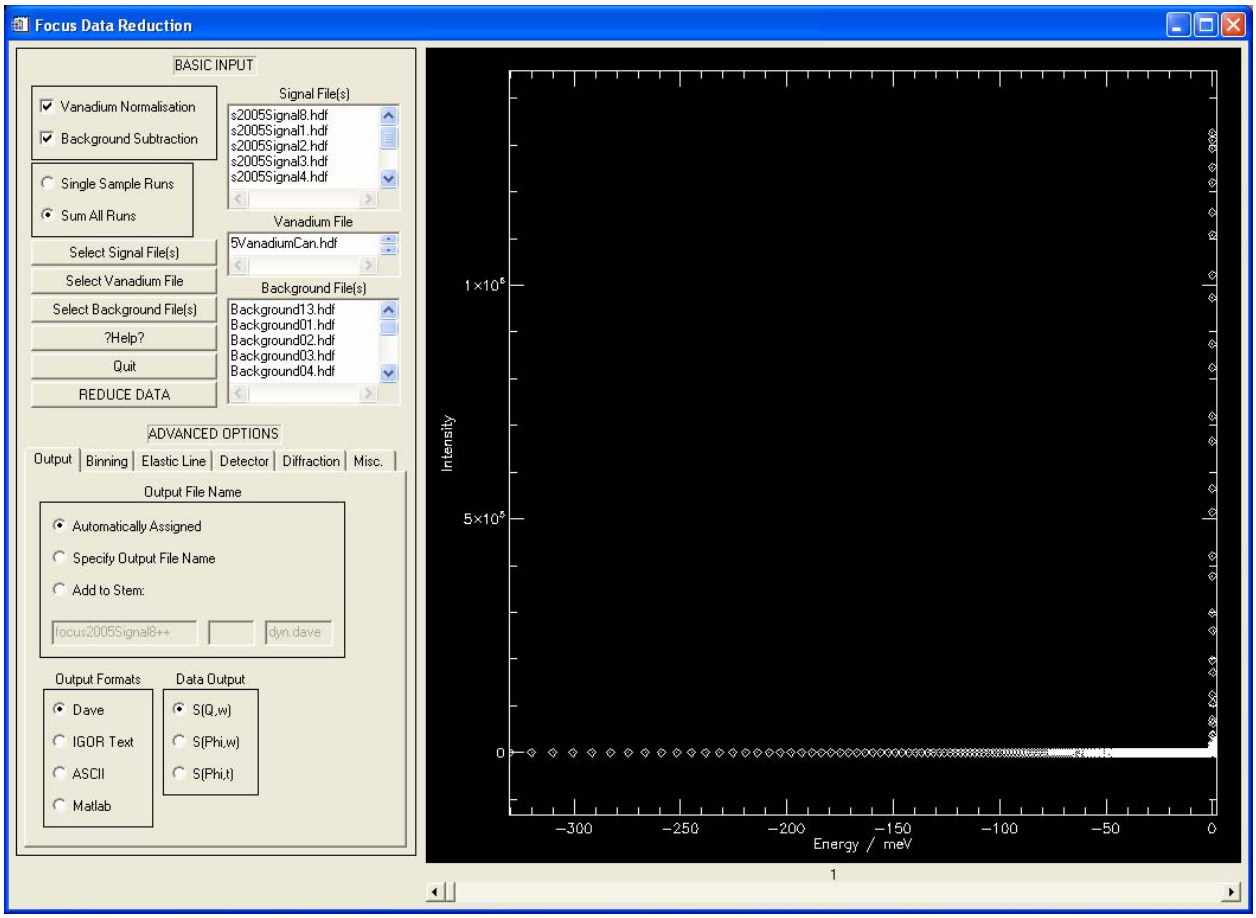
To initiate FDR, click on the Data Reduction Menu and move the mouse to select the program as follows:



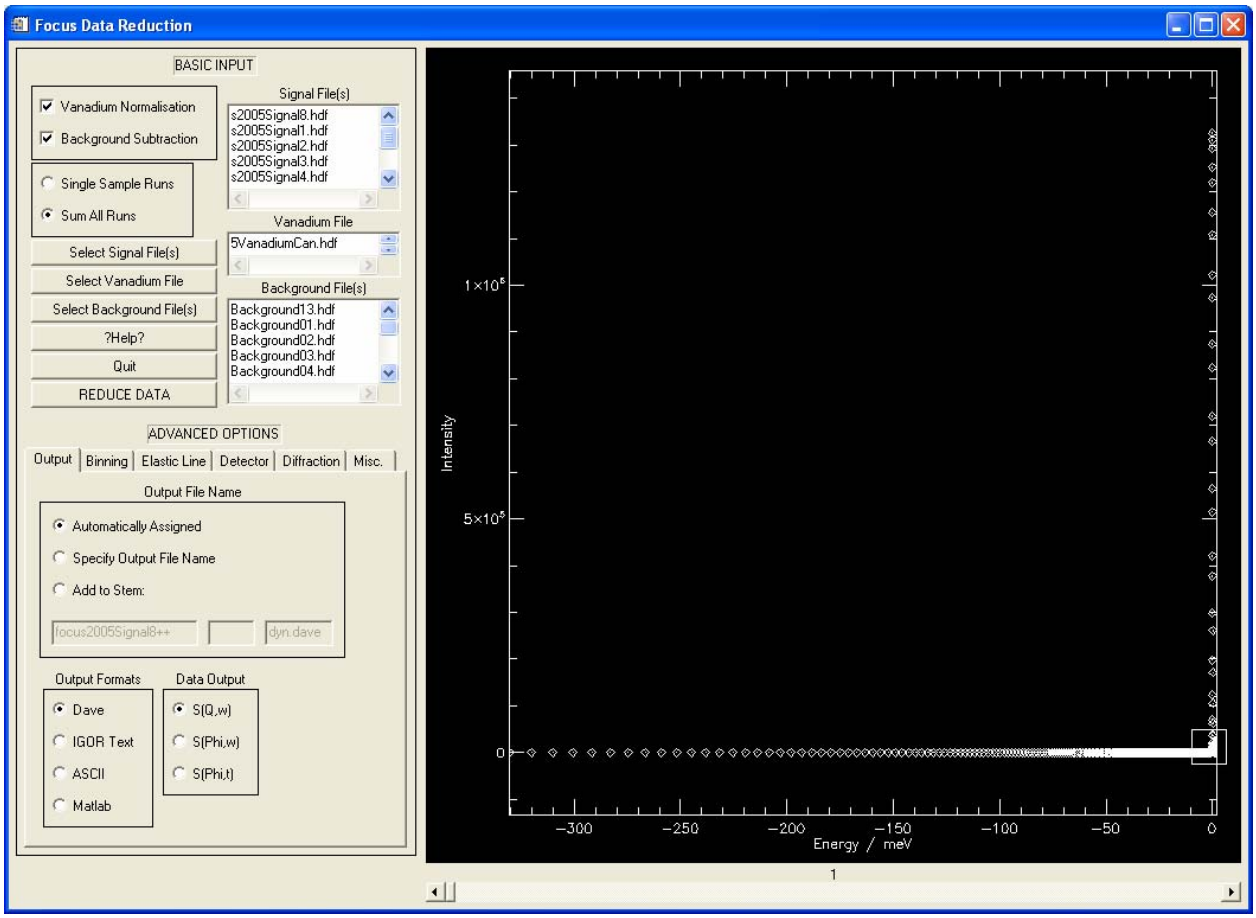
The main menu for the program should then appear:

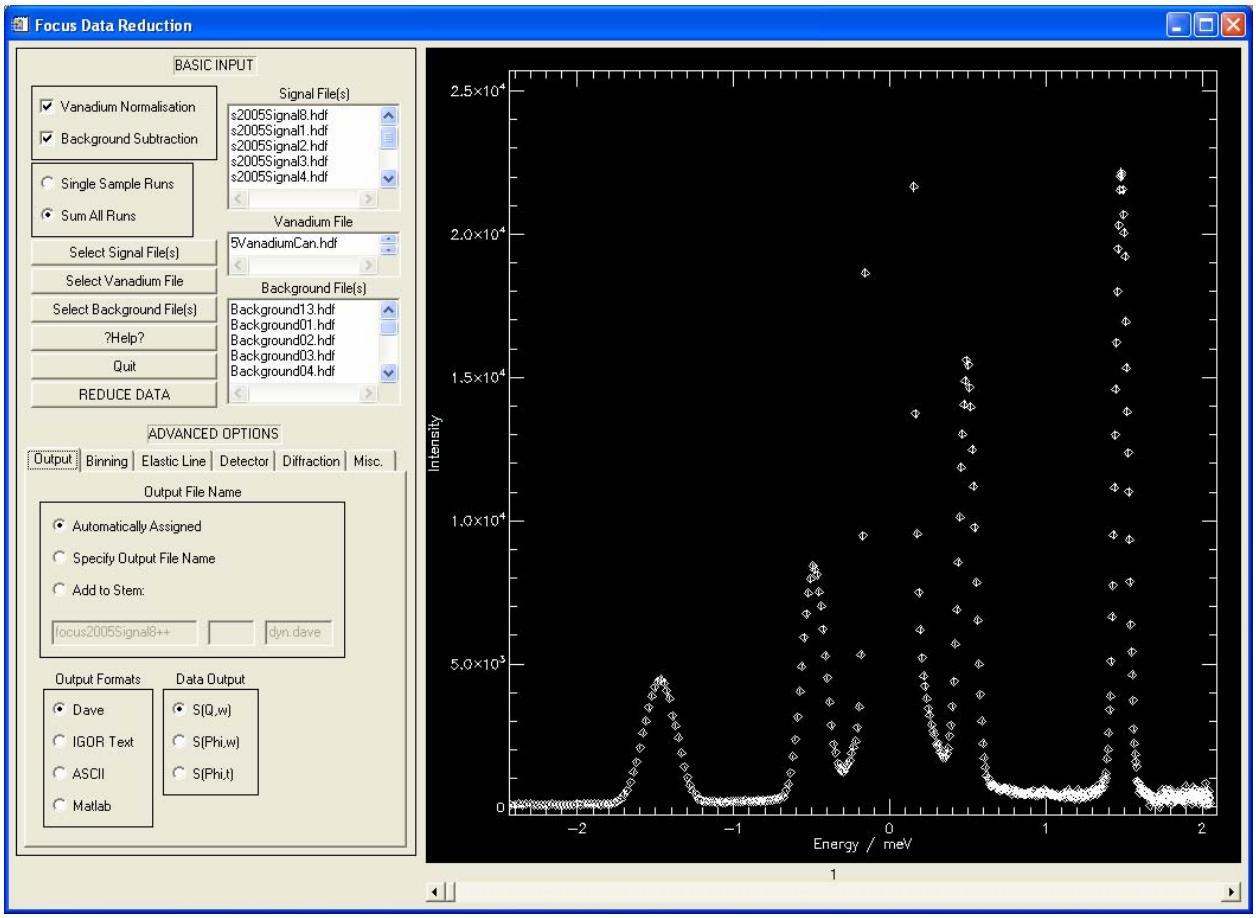


The interface was conceived with the idea of accommodating both the novice and the seasoned user. A data set can be reduced quickly and reliably by entering just the basic input, and allowing the program to choose the remaining settings. The only essential information required by the program is signal files. The basic input menu largely follows that written by Rob Dimeo for his HFBS reduction program, allowing the user to reduce a number of signal files individually (Single Sample Runs) or to sum the files together (Sum All Runs). Background files consist of data from the empty can. The files are automatically summed if more than one is present. The vanadium file consists of data from vanadium metal. When files in all three categories are selected, and the settings of the ADVANCED OPTIONS have not been altered, the action of pressing the "REDUCE DATA" button yields an output that should look something like this:



From inspection of the "Output" menu under "ADVANCED OPTIONS", it may be seen that the program has converted the raw data to S(Q,ω), and saved the output as a DAVE file, with the stem of the file name taken from the input signal file. The spectrum is plotted on the right-hand-side of the display window. The useful information is typically contained within a few meV of the exciting line. The user can zoom-in on the range of the spectrum of interest by creating a window using the mouse with the left button depressed and then releasing. A click of the right mouse button returns the view window to display the full range.


Focus Data Reduction
BASIC INPUT
Vanadium Normalisation
Background Subtraction
Single Sample Runs
Sum All Runs
Select Signal File(s)
Select Vanadium File
Select Background File(s)
?Help?
Quit
REDUCE DATA
Signal File(s)
s2005Signal8.hdf
s2005Signal1.hdf
s2005Signal2.hdf
s2005Signal3.hdf
s2005Signal4.hdf
Vanadium File
5VanadiumCan.hdf
Background File(s)
Background13.hdf
Background01.hdf
Background02.hdf
Background03.hdf
Background04.hdf
ADVANCED OPTIONS
Output
Binning
Elastic Line
Detector
Diffraction
Misc.
Output File Name
Automatically Assigned
Specify Output File Name
Add to Stem:
focus2005Signal8++
dyn.dave
Output Formats
Dave
IGOR Text
ASCII
Matlab
Data Output
S(Q,w)
S(Phi,w)
S(Phi,t)
Intensity
1×10⁵
5×10⁵
0
−300
−250
−200
−150
−100
−50
0
Energy / meV
1

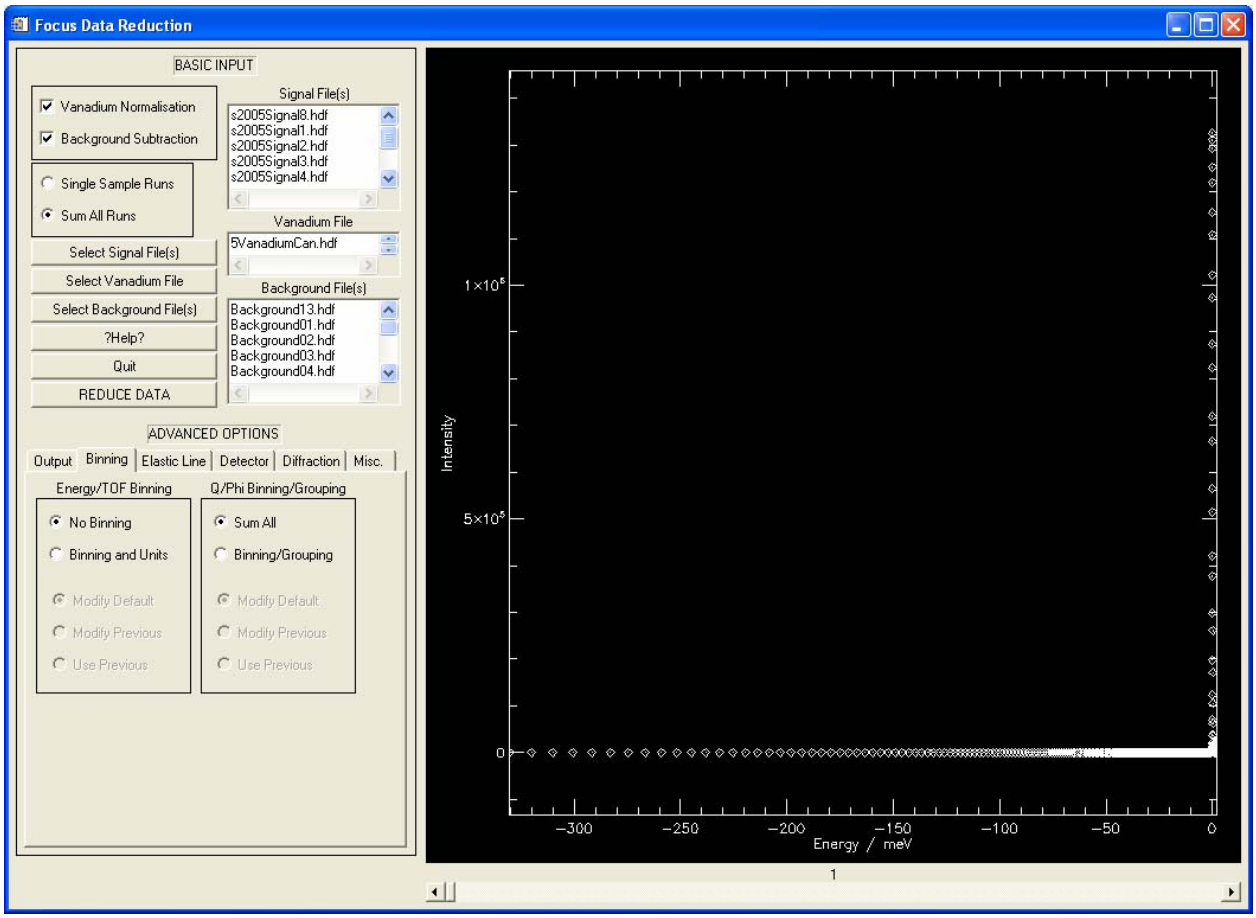


The remaining default settings may be inspected by clicking on the tabs under "ADVANCED OPTIONS".

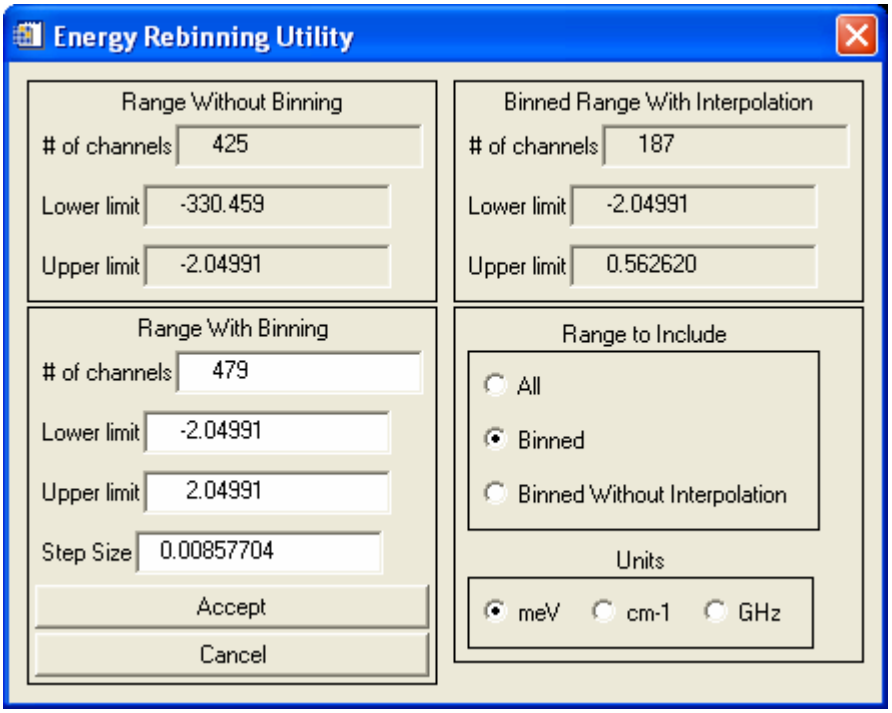
3. Advanced Program Options

In this section, details are given on those Advanced Options that are not self-explanatory.

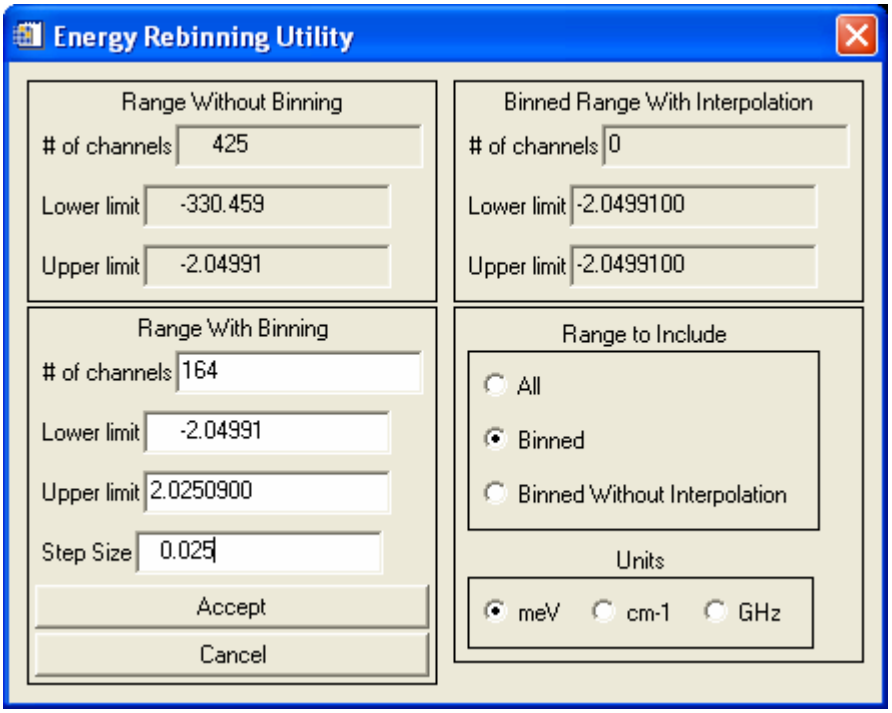
The default is no energy binning with the data summed over all detectors.



When the “Binning and Units” option is selected under “Energy/TOF Binning”, the following menu appears during the reduction process:

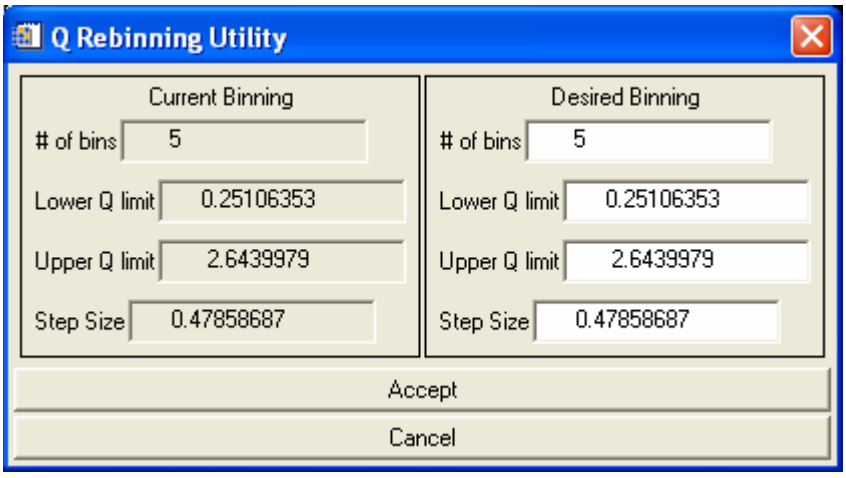


The energy range is divided into regions with and without binning. The binned region is further divided into regions with and without interpolation. All fields are automatically updated by changing one of the editable fields and then pressing the carriage return. The total number of output channels cannot exceed the total number of input channels. If binned data are required over a wide energy range, but interpolation is not desired, the step size should be increased, and/or the number of channels decreased, until the interpolation range diminishes to zero.

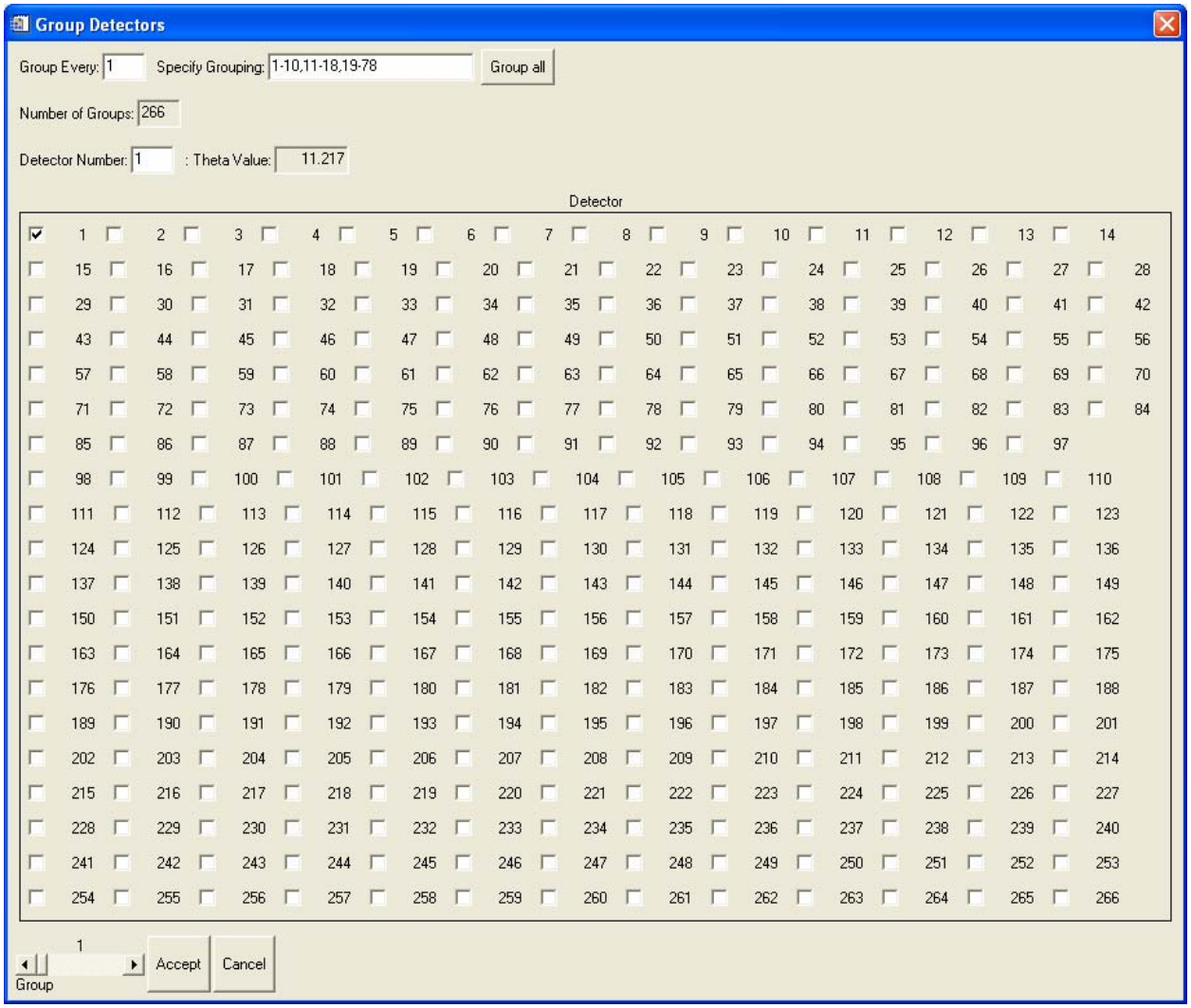


The default is to sum the data summed over all detectors. If Q binning is desired then "Binning/Grouping" under "Q/Phi Binning/Grouping" should be selected. Before attempting to calculate the Q dependence, the user should know the accessible Q-range for the transition in question. This may be determined using the DAVE neutron calculator facility, which is to be found under the "Planning" menu.

When Q binning is selected the following dialogue appears:

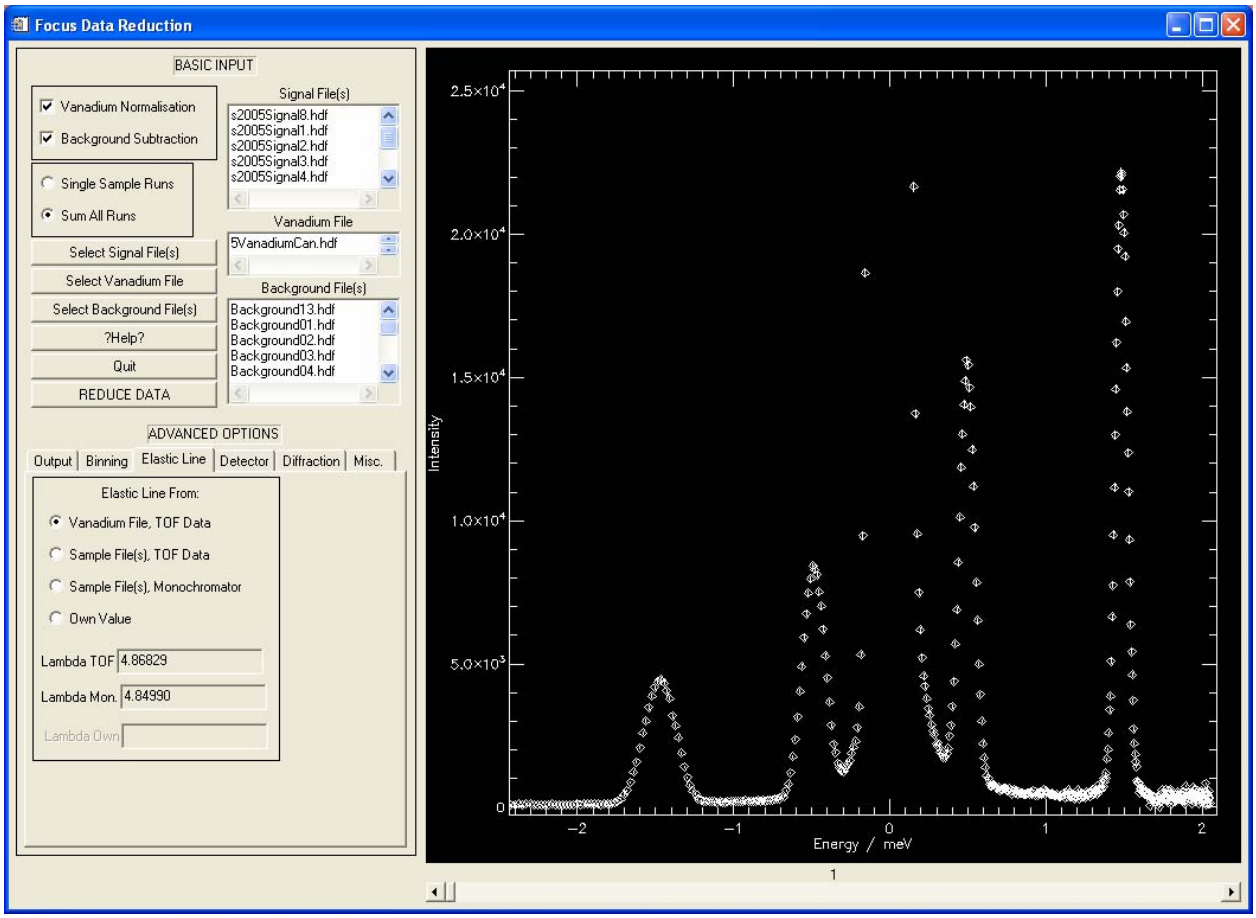


Press the carriage return after modifying a given editable field. If the quantity to be calculated is not S(Q,ω) but S(phi,ω) then checking the "Binning/Grouping" box under "Q/Phi Binning/Grouping" results in the following dialogue appearing during the reduction process:

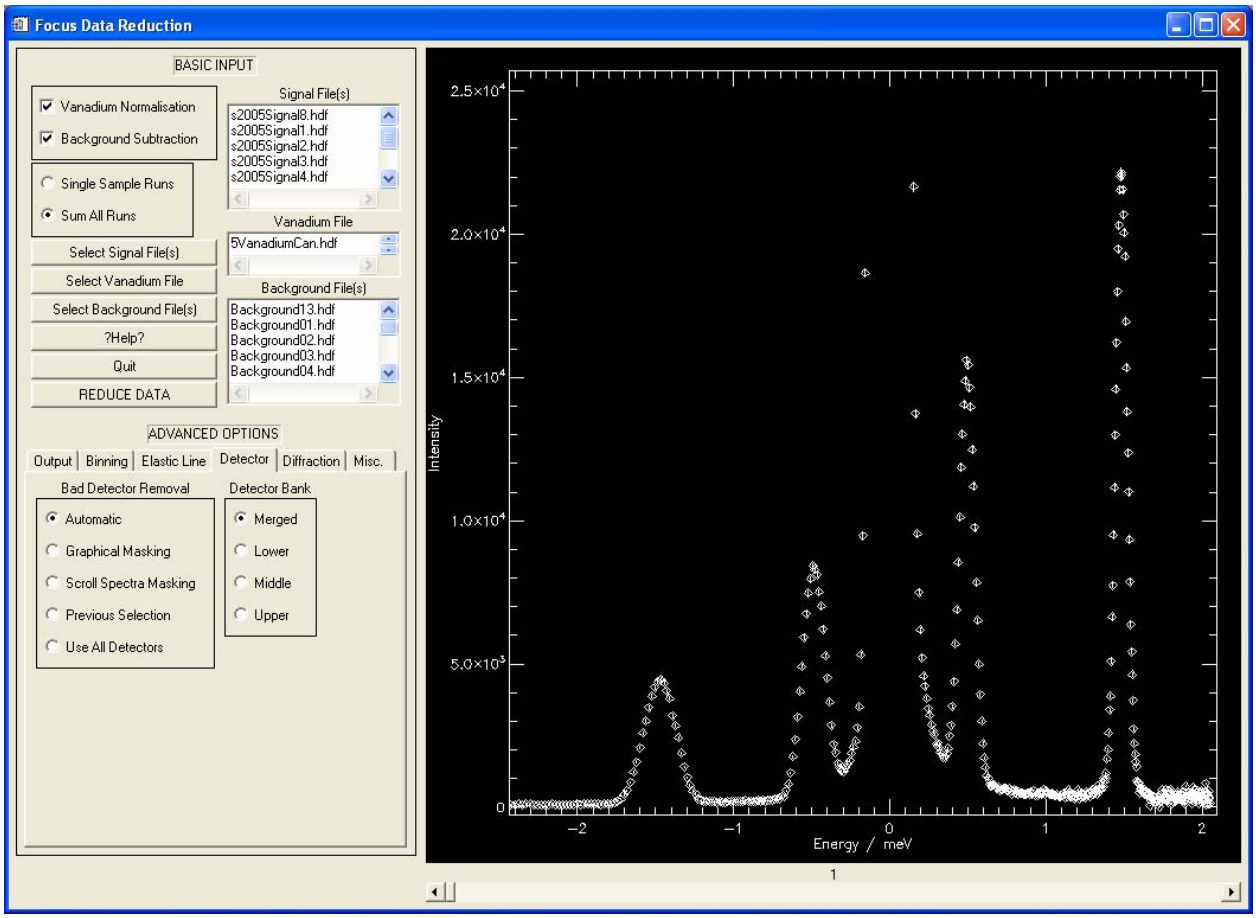


The detectors may be grouped in three different ways: By entering a value in the "Group Every" field and pressing the carriage return; by entering a string in the "Specify Grouping" field, paying attention to the format in the example; and finally by checking the boxes for a given group. The detectors selected in a given group may be viewed by moving the slider bar appropriately.

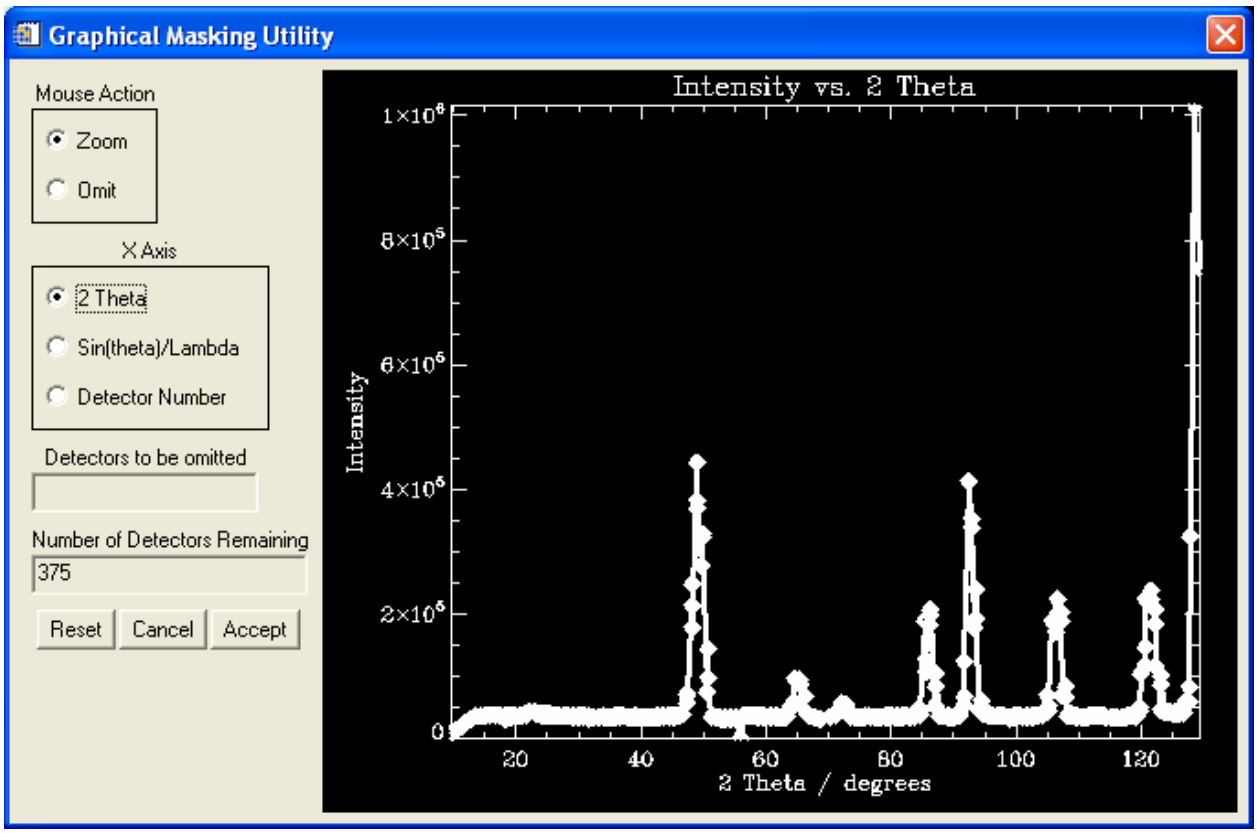
The elastic line will be calculated from the vanadium file unless otherwise specified. If no vanadium file is selected then the default is to calculate the elastic line from the signal data. During the reduction process, the value of lambda, calculated from time-of-flight data will be displayed. This should be similar to the value calculated from the monochromator position.



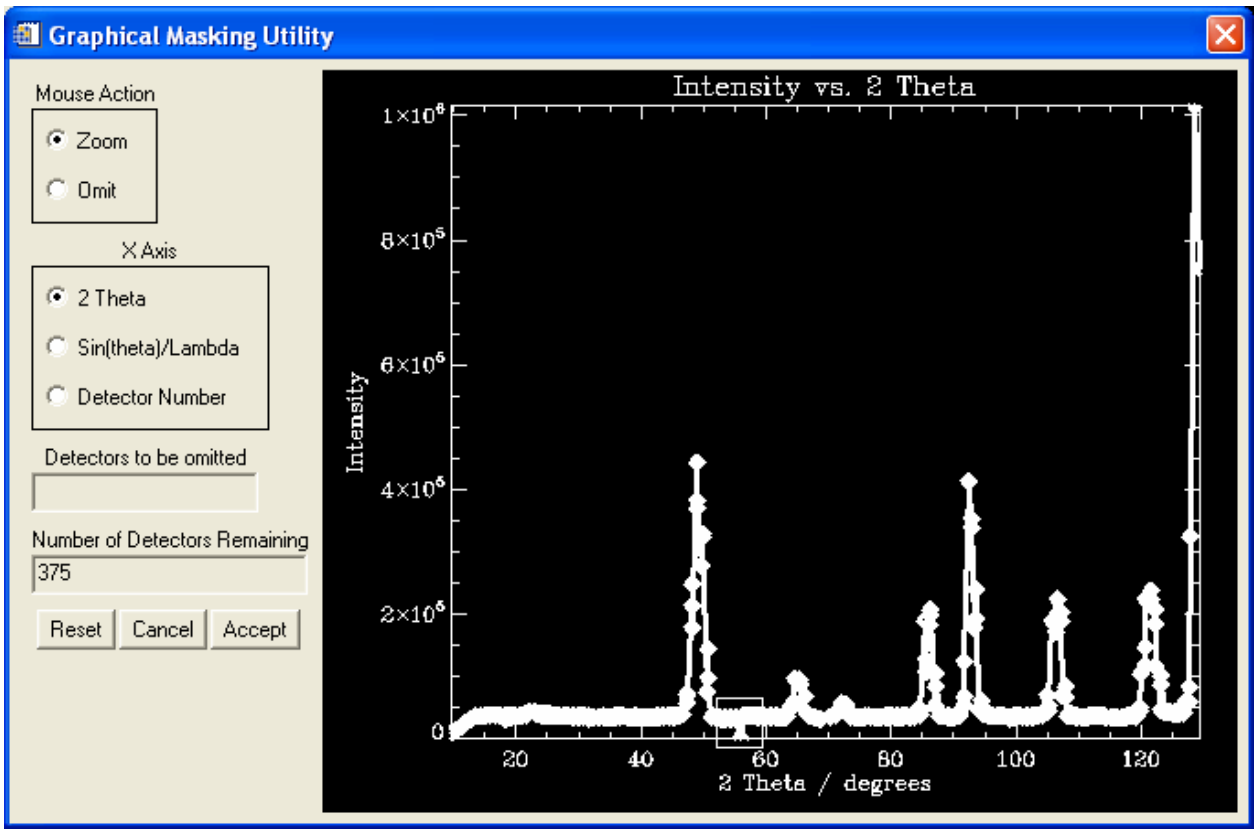
The automatic bad detector removal option removes all detectors with a signal less than a 20% percentage of the average. It is especially important to remove dead detectors, as the program will crash if these detectors are not removed and the program tries to correct for variable detector efficiency. There are three detector banks: upper, middle and lower. The default “merged” option is self-explanatory.

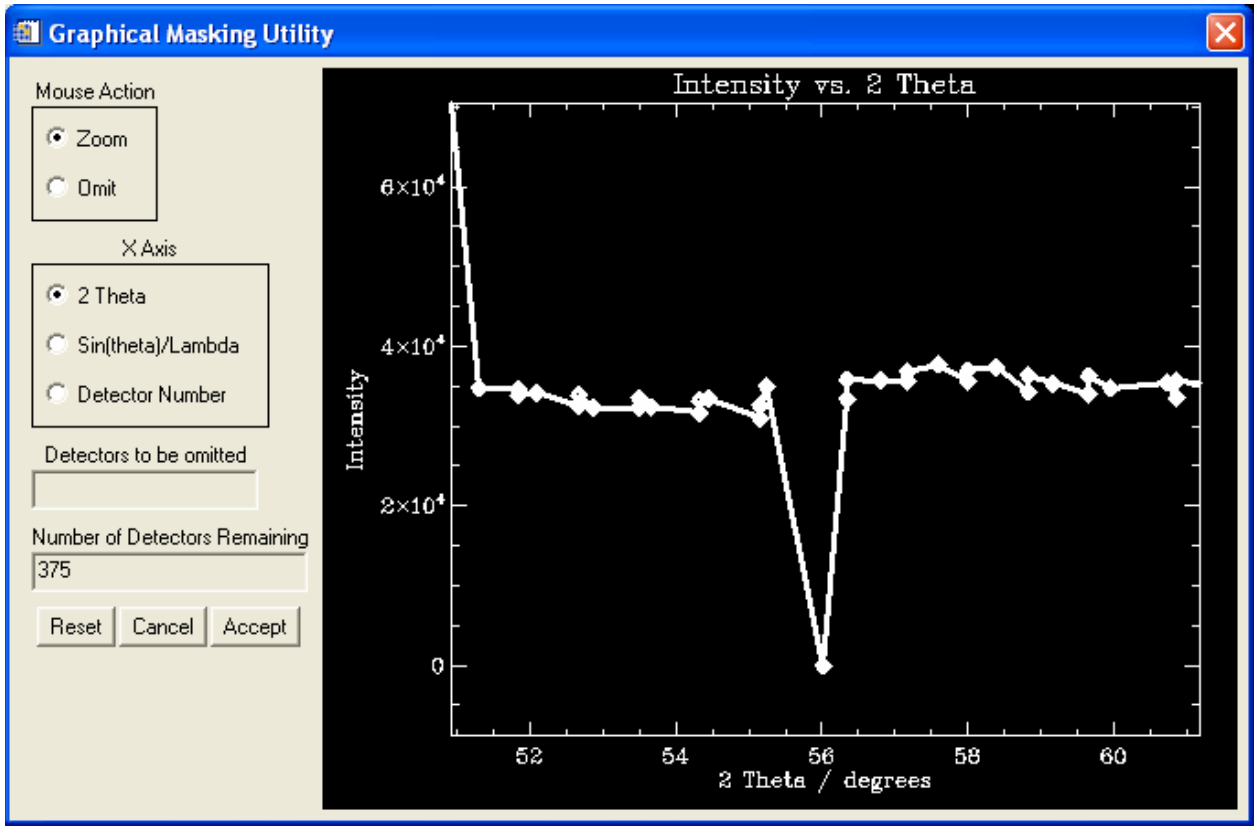


The Graphical Masking and Scroll Spectra Masking tools allow the user to remove certain detectors manually during the reduction process. If the Graphical Masking option is chosen, the following dialogue appears during the reduction process:

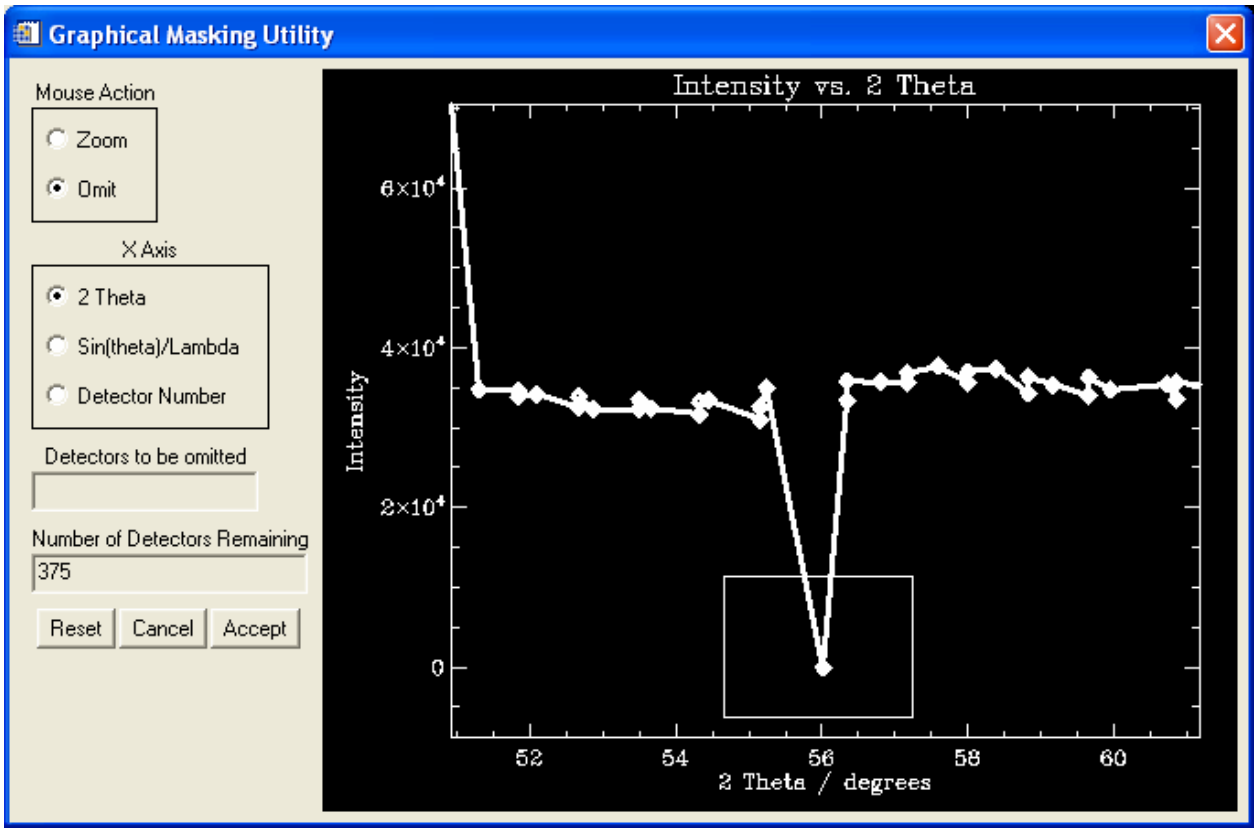


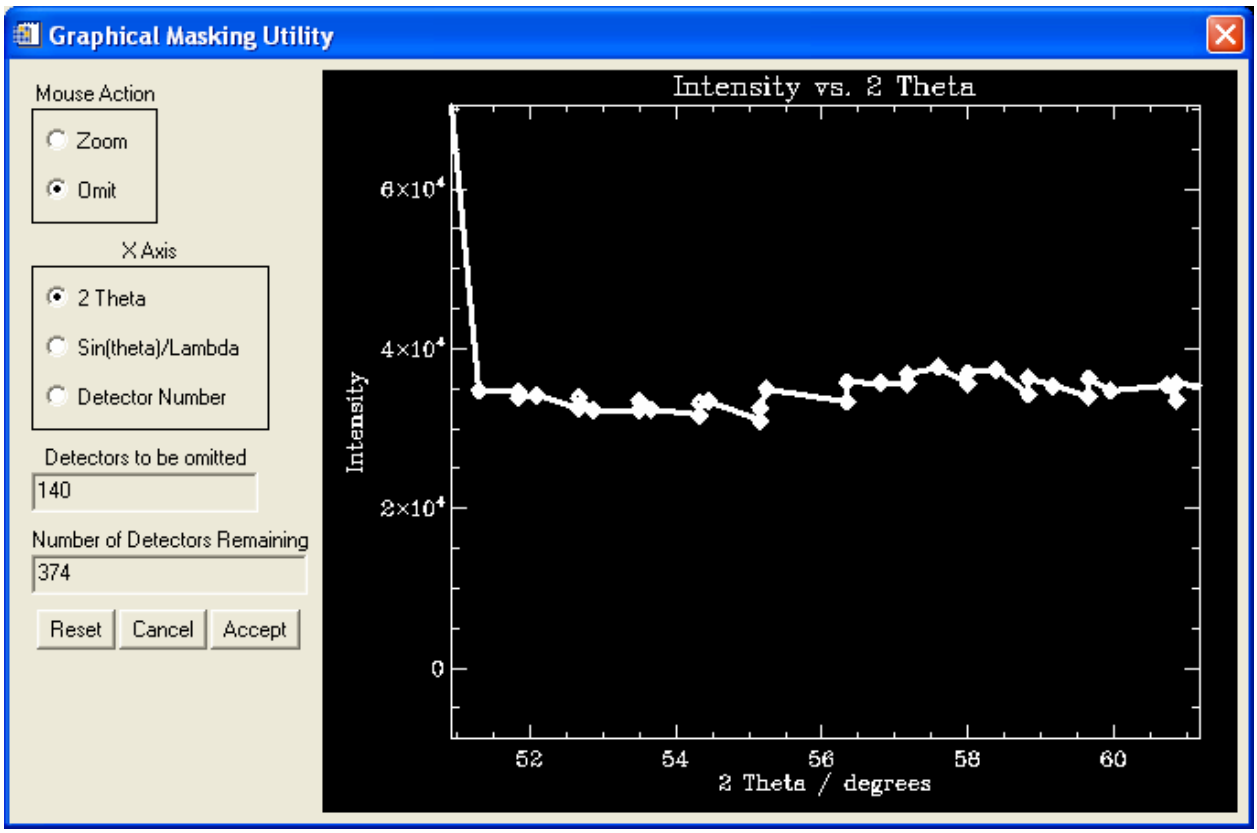
The data may be plotted as a function of 2 Theta, Sin(theta)/lambda or detector number. Be aware that some detectors will have the same value of theta, when housed in different detector banks. Zoom into the area of interest using the mouse.


Graphical Masking Utility
Mouse Action
Zoom
Omit
X Axis
2 Theta
Sin(theta)/Lambda
Detector Number
Detectors to be omitted
Number of Detectors Remaining
375
Reset
Cancel
Accept
Intensity vs. 2 Theta
Intensity
2 Theta / degrees


Graphical Masking Utility
Mouse Action
Zoom
Omit
X Axis
2 Theta
Sin(theta)/Lambda
Detector Number
Detectors to be omitted
Number of Detectors Remaining
375
Reset
Cancel
Accept
Intensity vs. 2 Theta
Intensity
2 Theta / degrees

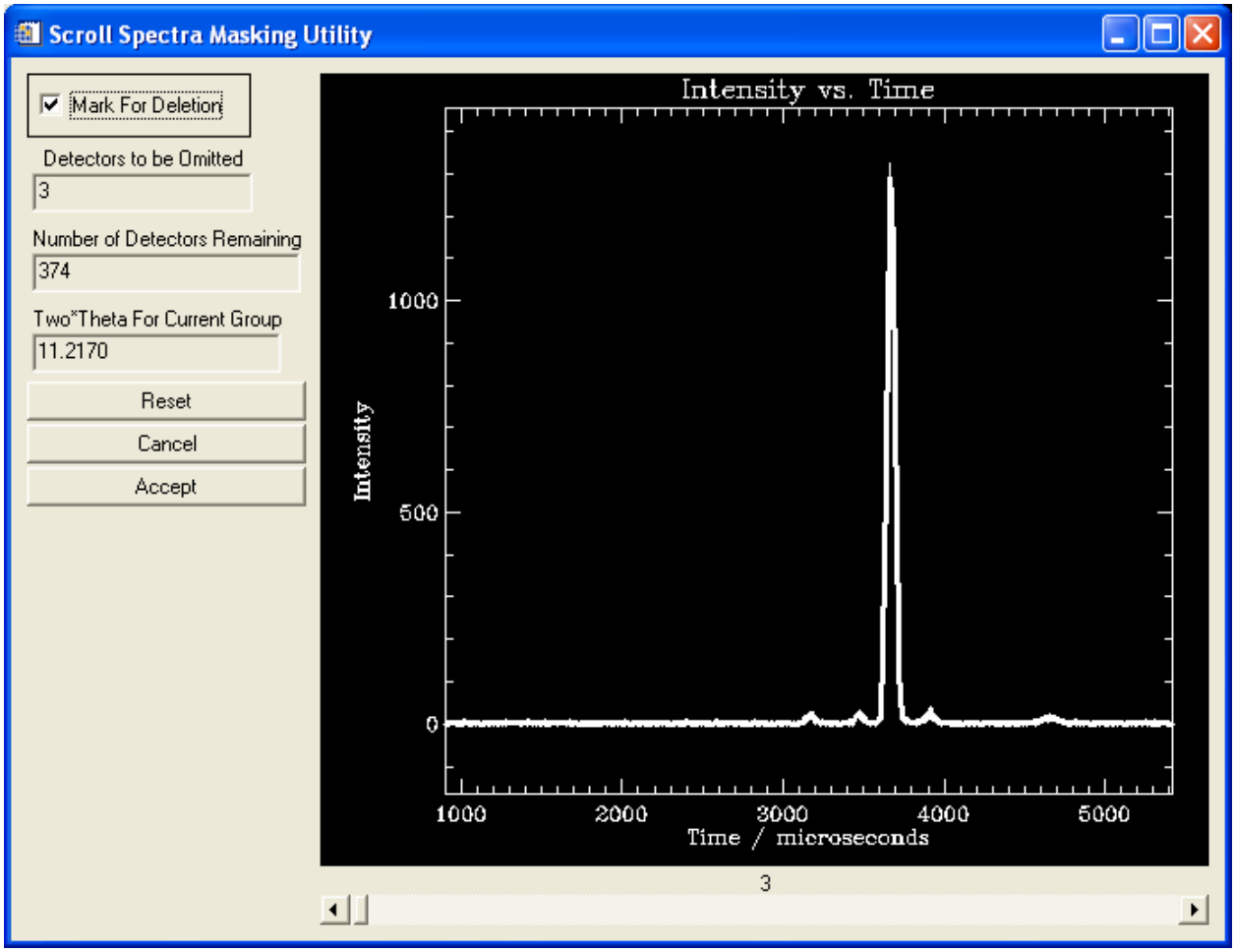
Next, change the mouse action to omit. Detectors, whose intensity and x value are enclosed within the window defined by the mouse, will now be removed:





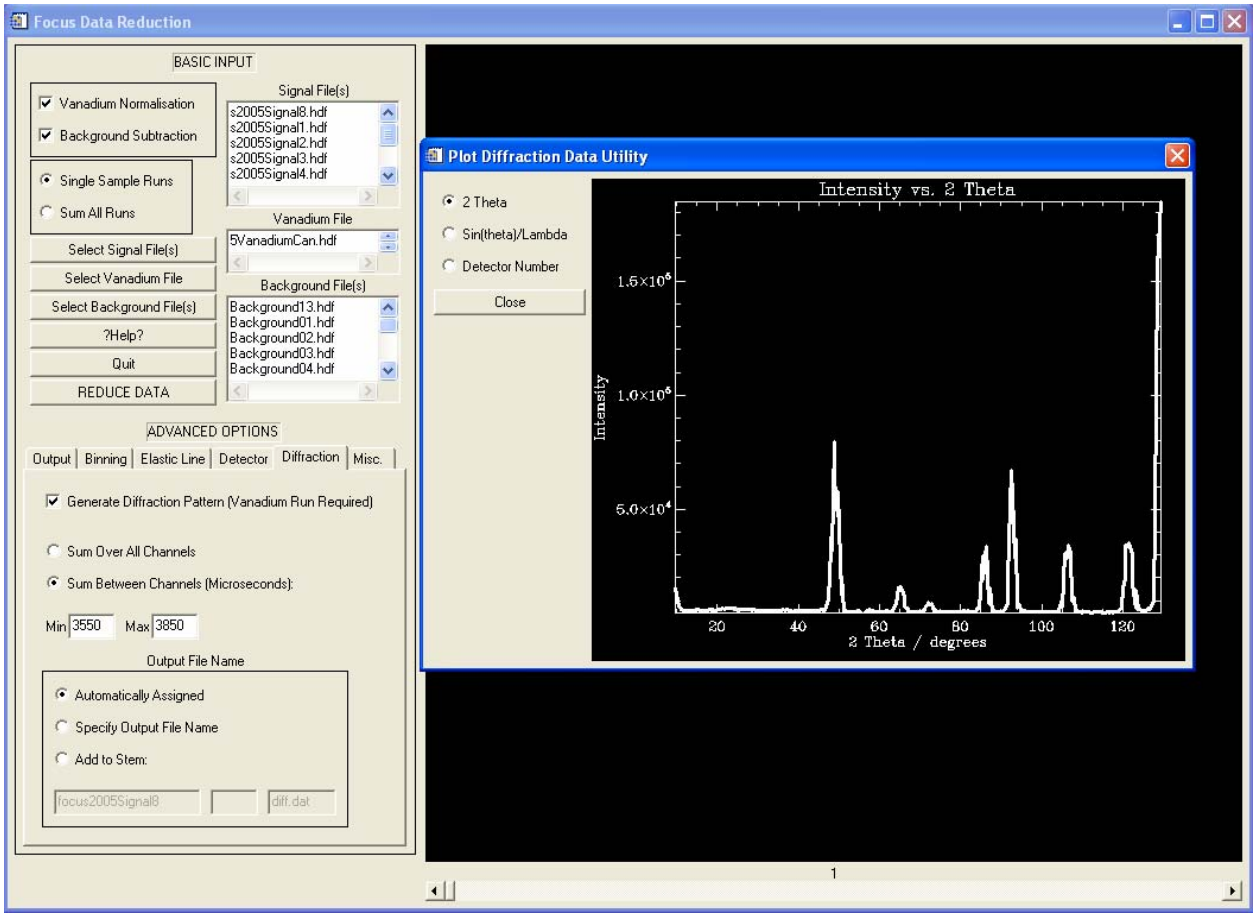
Press “Accept” when completed.

By contrast, the Scroll Spectra Masking option allows the user to view the raw data for each detector.



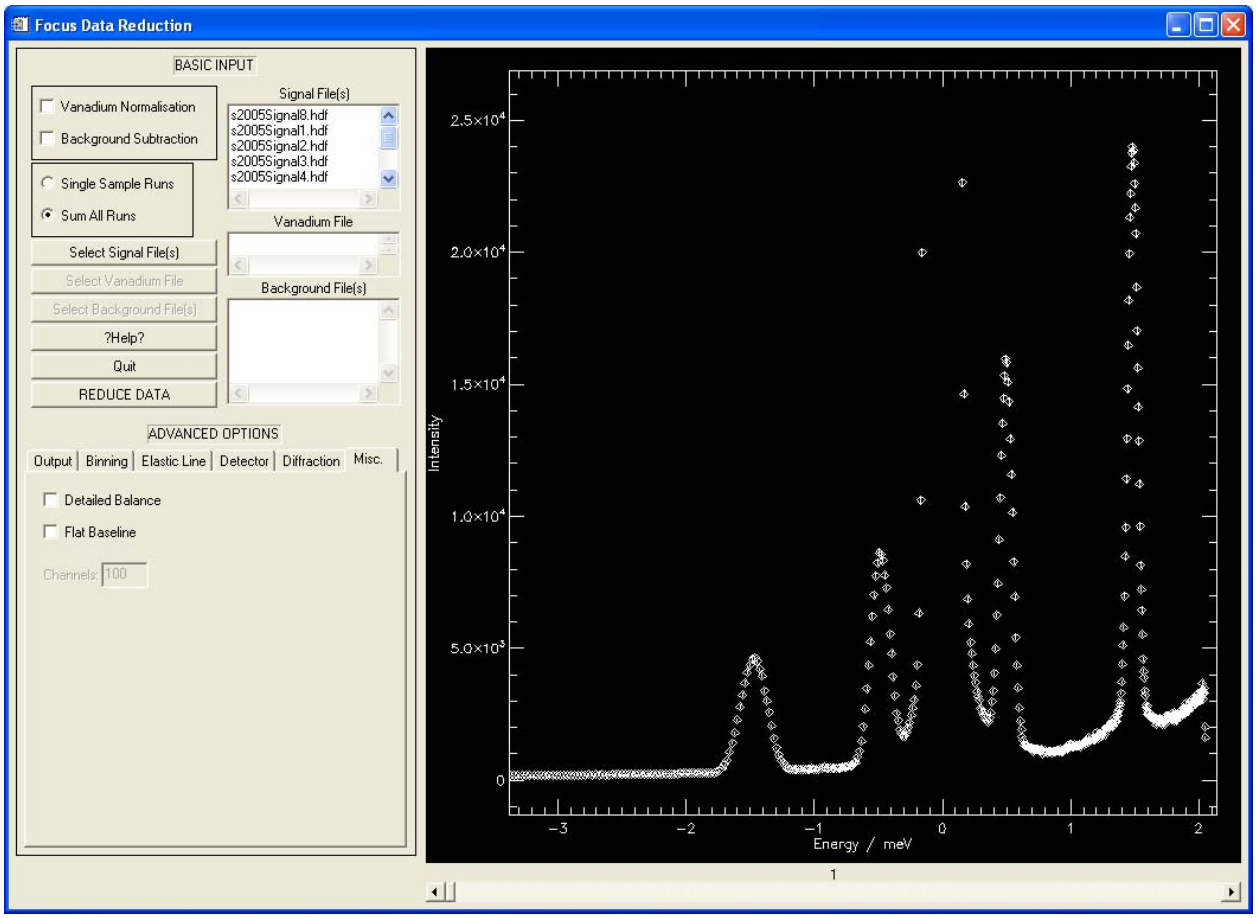
The data from a given detector may be viewed by moving the slider bar appropriately. Those detectors marked for deletion will be removed when the Accept button is pressed.

A low-resolution diffraction pattern may be calculated from data collected on the FOCUS instrument. In order for the intensities to be meaningful, the detectors must be calibrated using data from a vanadium run. The intensities may be calculated either from the sum over all channels, or from channels in a given time window. The latter option is preferable when inelastic transitions are strong. The diffraction pattern is plotted during the reduction process and a file containing the data is created.

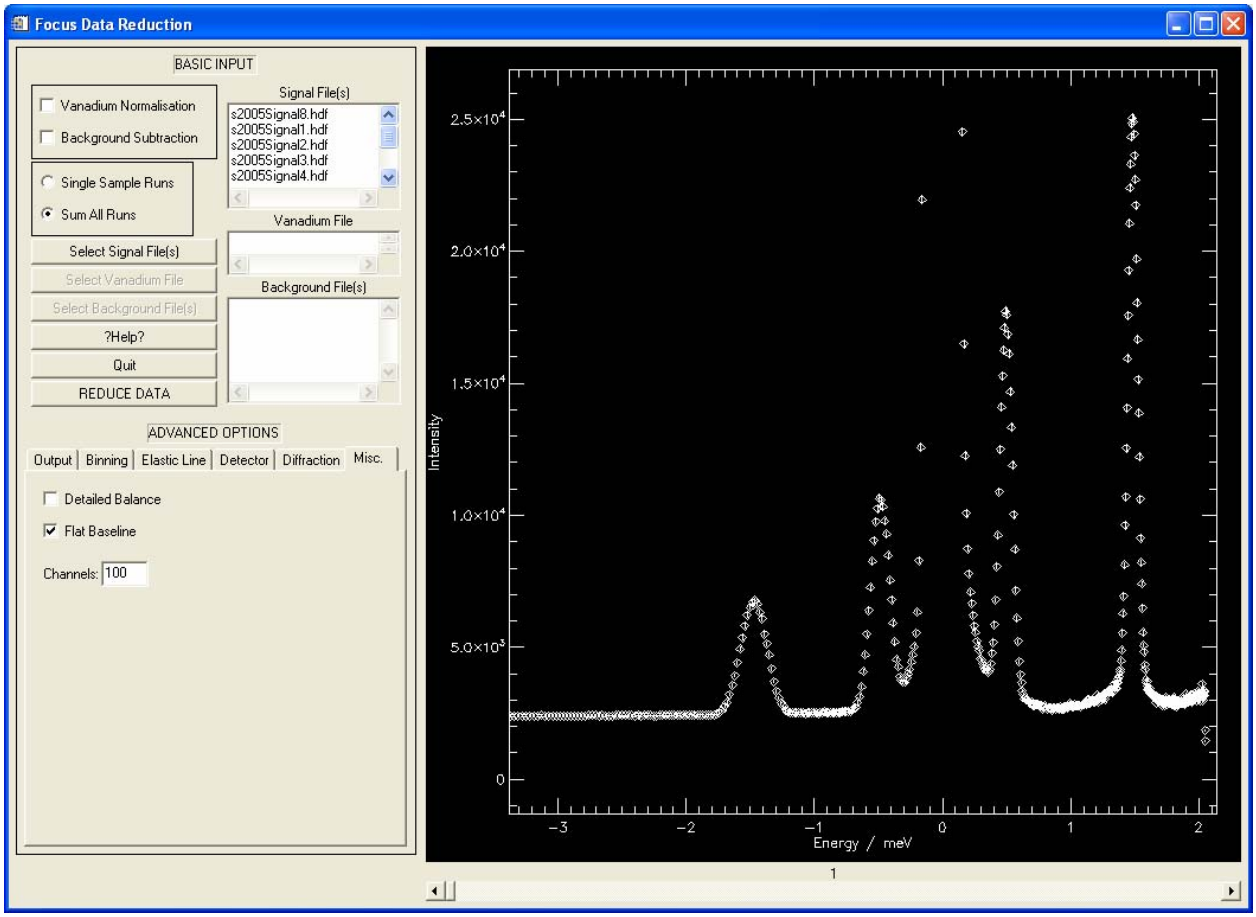


If the Detailed Balance option is selected under the Misc. tab, the data are multiplied by the factor $e^{-E/2kT}$. The "correction" is appropriate only for excitations obeying Bose statistics, phonons for example.

If data of the empty can were not collected, then the baseline can be fiddled using the flat baseline option, also to be found under the Misc. tab. With no background subtraction, the baseline is seen to rise steeply on the neutron energy loss side of the spectrum:

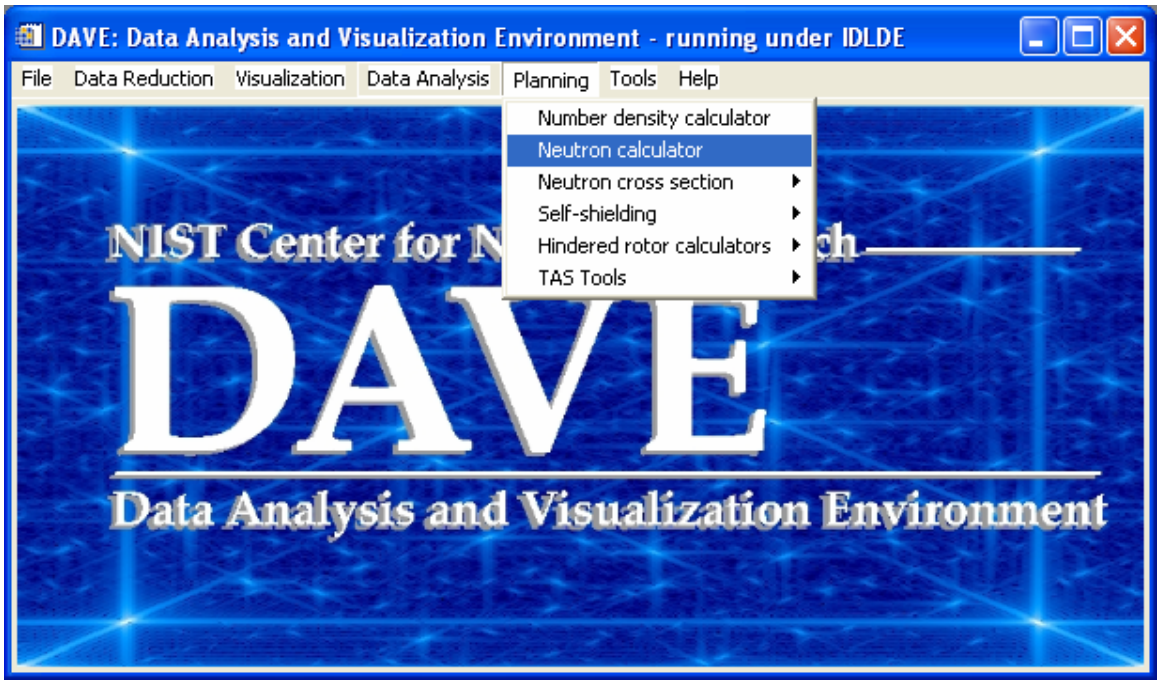


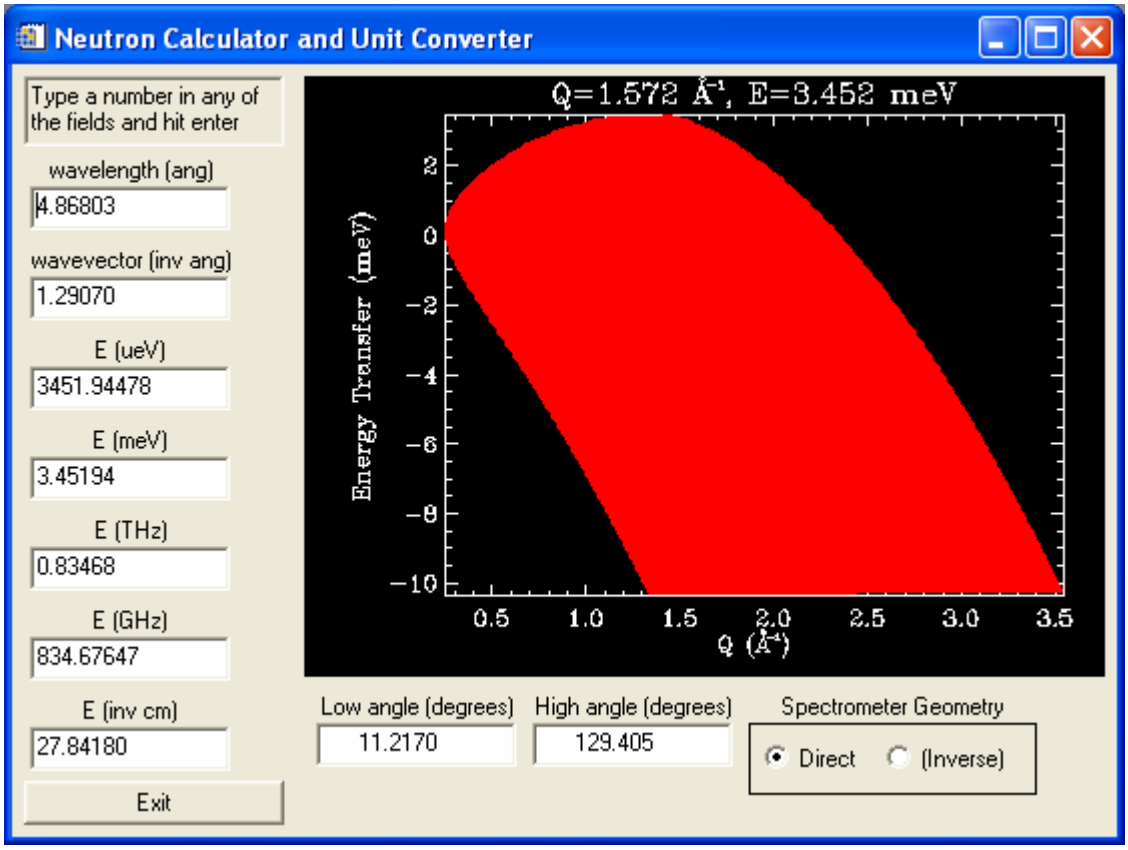
This is because the conversion from time to energy incorporates an intensity correction of t_f^4, where t_f is the time-of-flight from the sample to the detector. The flat baseline option subtracts a constant from all the raw data before conversion to energy. This constant is calculated as follows: The mean number of counts is calculated successively over a given number of channels. In the example shown below, 100 channels. If there are 904 channels, then 10 mean values are calculated. The lowest mean value is the constant to be subtracted from all the data. By removing this offset, a flat baseline can be obtained



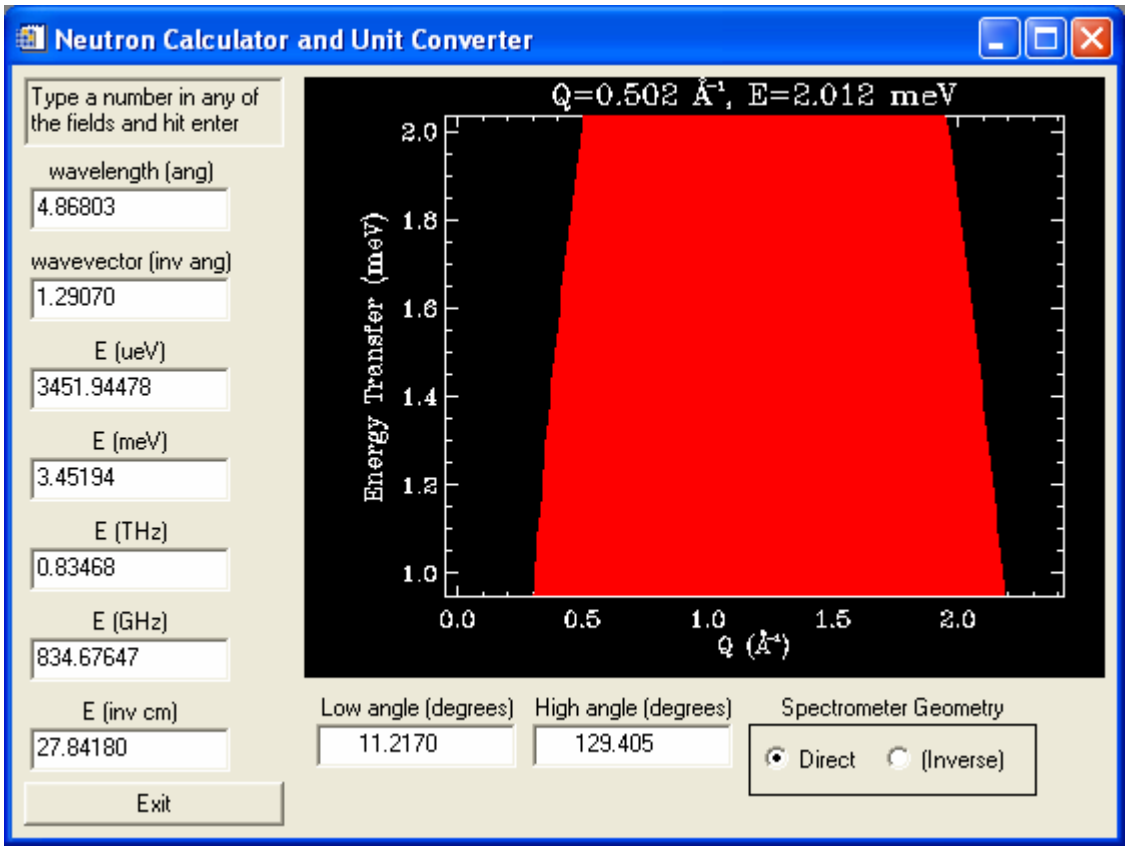
4. A Working Example

In this section, the steps that the user might take to reduce his data set, and calculate the Q-dependence of a given transition, are described. Let us calculate the Q-dependence of the intensity of the high-energy transition in the spectrum above. The first step is to know the accessible Q-range for the transition in question. This is determined by the energy of the incoming neutrons and the range of detector angles. Start the DAVE neutron calculator as shown, and enter the approproate values.

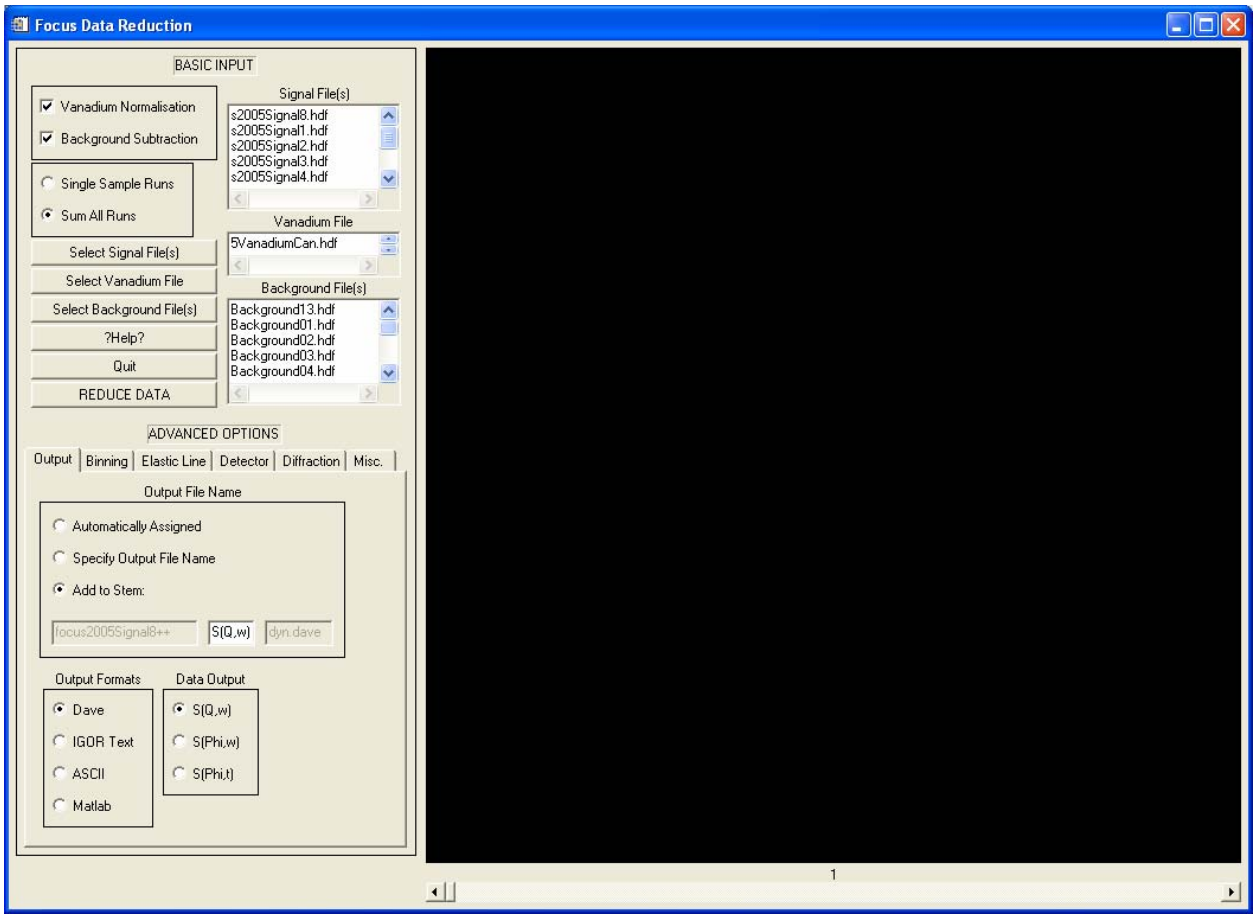

DAVE: Data Analysis and Visualization Environment - running under IDLDE
File
Data Reduction
Visualization
Data Analysis
Planning
Tools
Help
Number density calculator
Neutron calculator
Neutron cross section
Self-shielding
Hindered rotor calculators
TAS Tools
NIST Center for N ch
DAVE
Data Analysis and Visualization Environment


Neutron Calculator and Unit Converter
Type a number in any of the fields and hit enter
wavelength (ang)
4.86803
wavevector (inv ang)
1.29070
E (ueV)
3451.94478
E (meV)
3.45194
E (THz)
0.83468
E (GHz)
834.67647
E (inv cm)
27.84180
Exit
Q=1.572 Å⁻¹, E=3.452 meV
Energy Transfer (meV)
Q (Å⁻¹)
Low angle (degrees)
11.2170
High angle (degrees)
129.405
Spectrometer Geometry
Direct
(Inverse)

The red section shows the accessible Q-range. For a transition falling in the 1 to 2 meV energy range, the detectors cover a Q range from ca. 0.5 to 2.0 $Å^{-1}$.

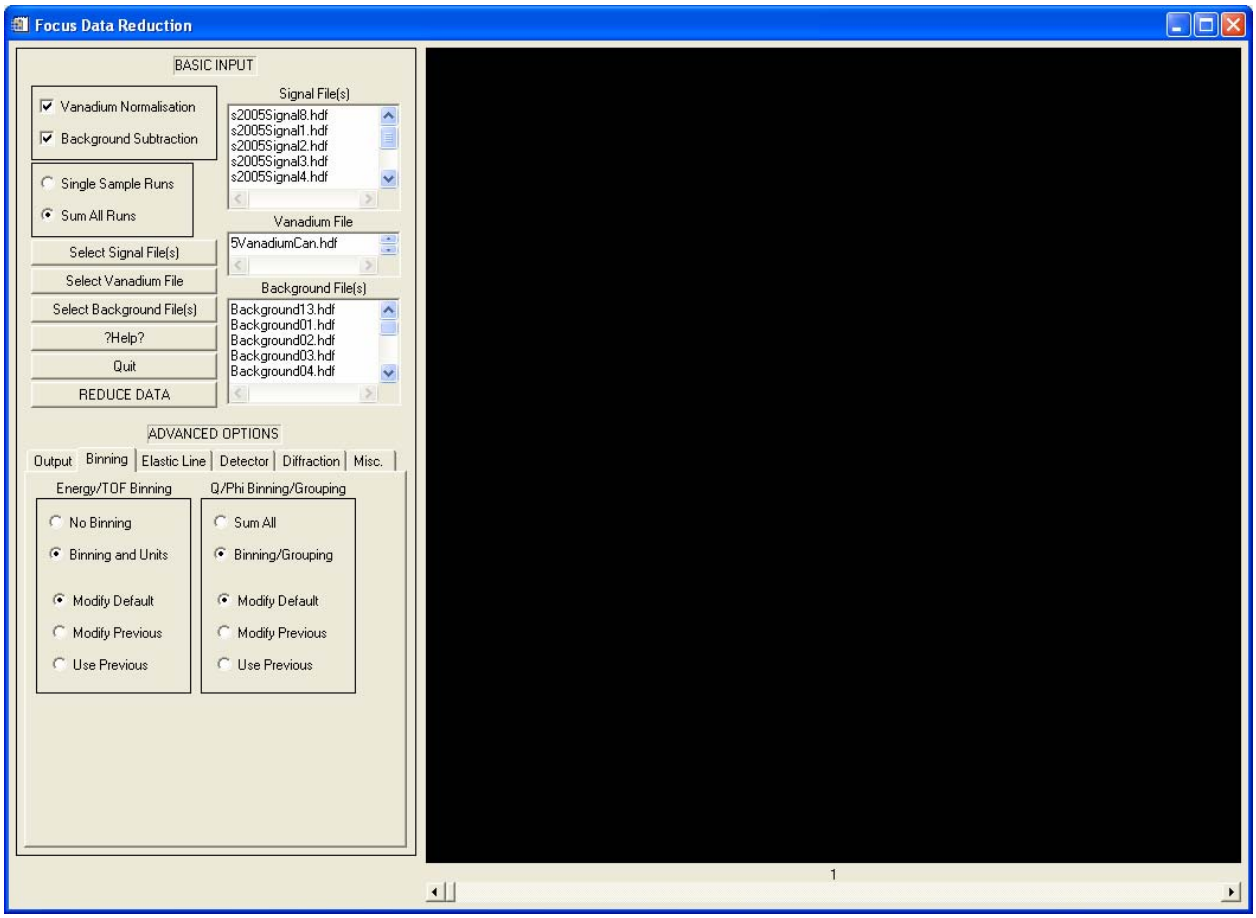


Next, we can reduce the data using the FOCUS Reduction program. A total of eight signal files were collected at 6 K for the sample of interest. We want to sum these files, subtract the background spectrum and calibrate the detectors with a vanadium file.

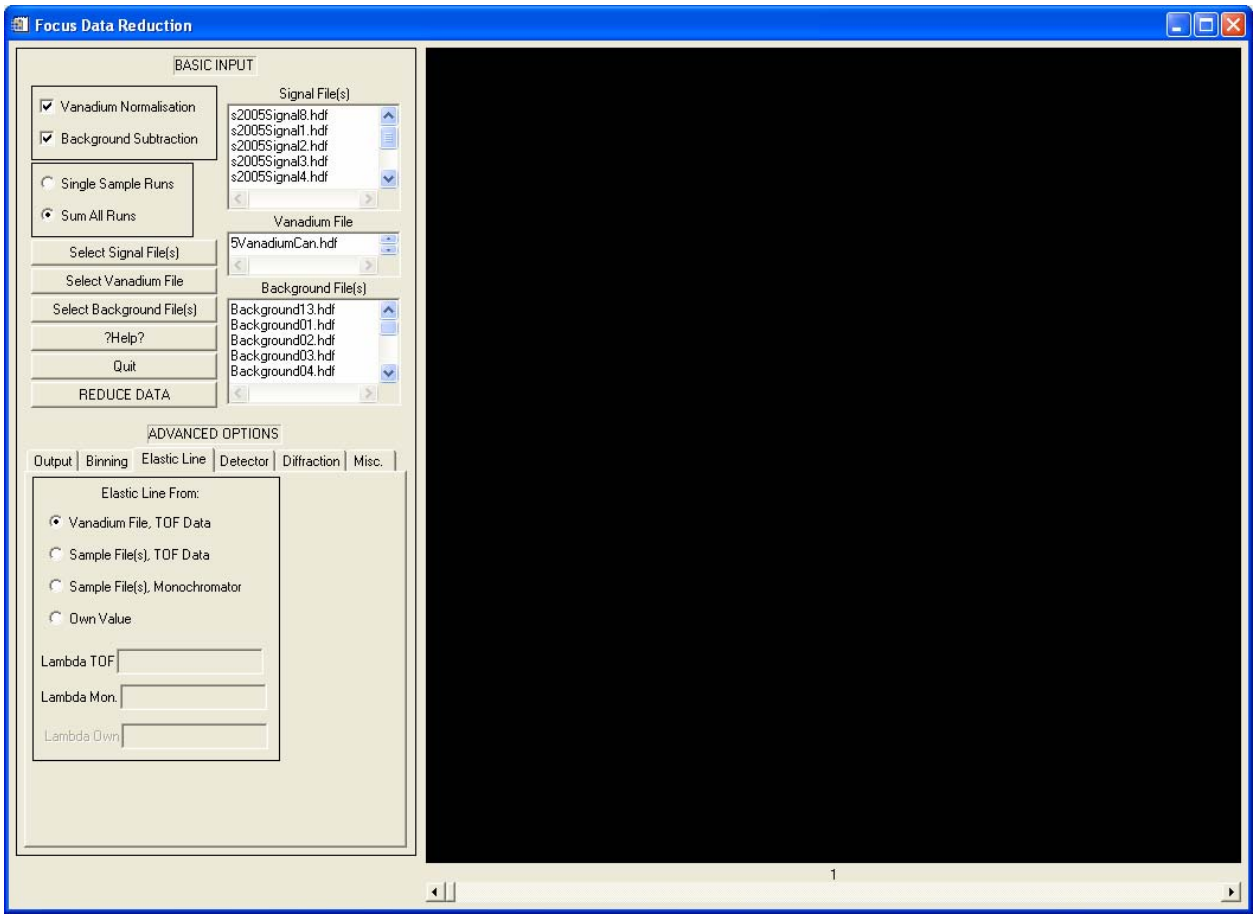


Returning to FDR, we have added S(Q,w) to the stem of the file name, to remind us of the data output we have specified.

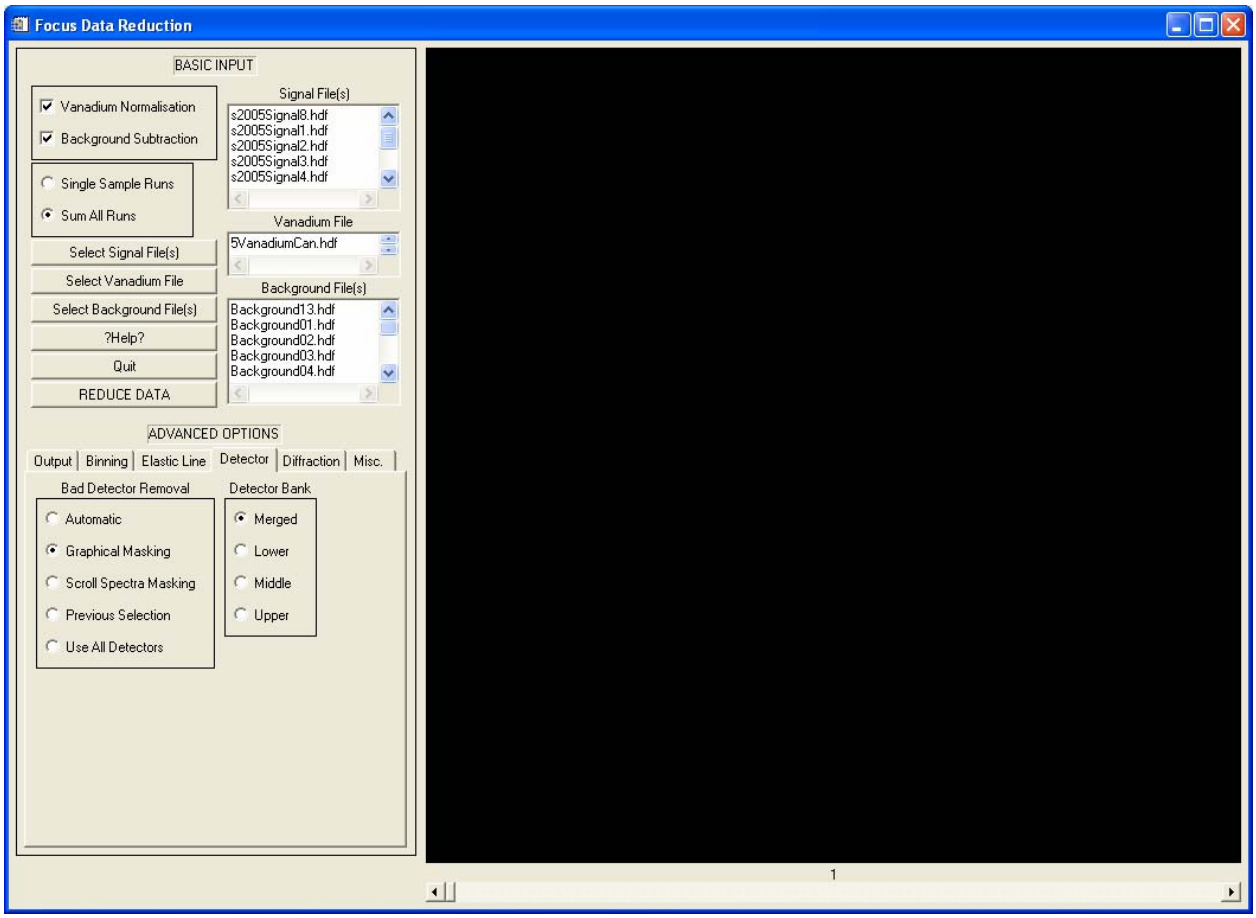
Both energy and Q binning are required:



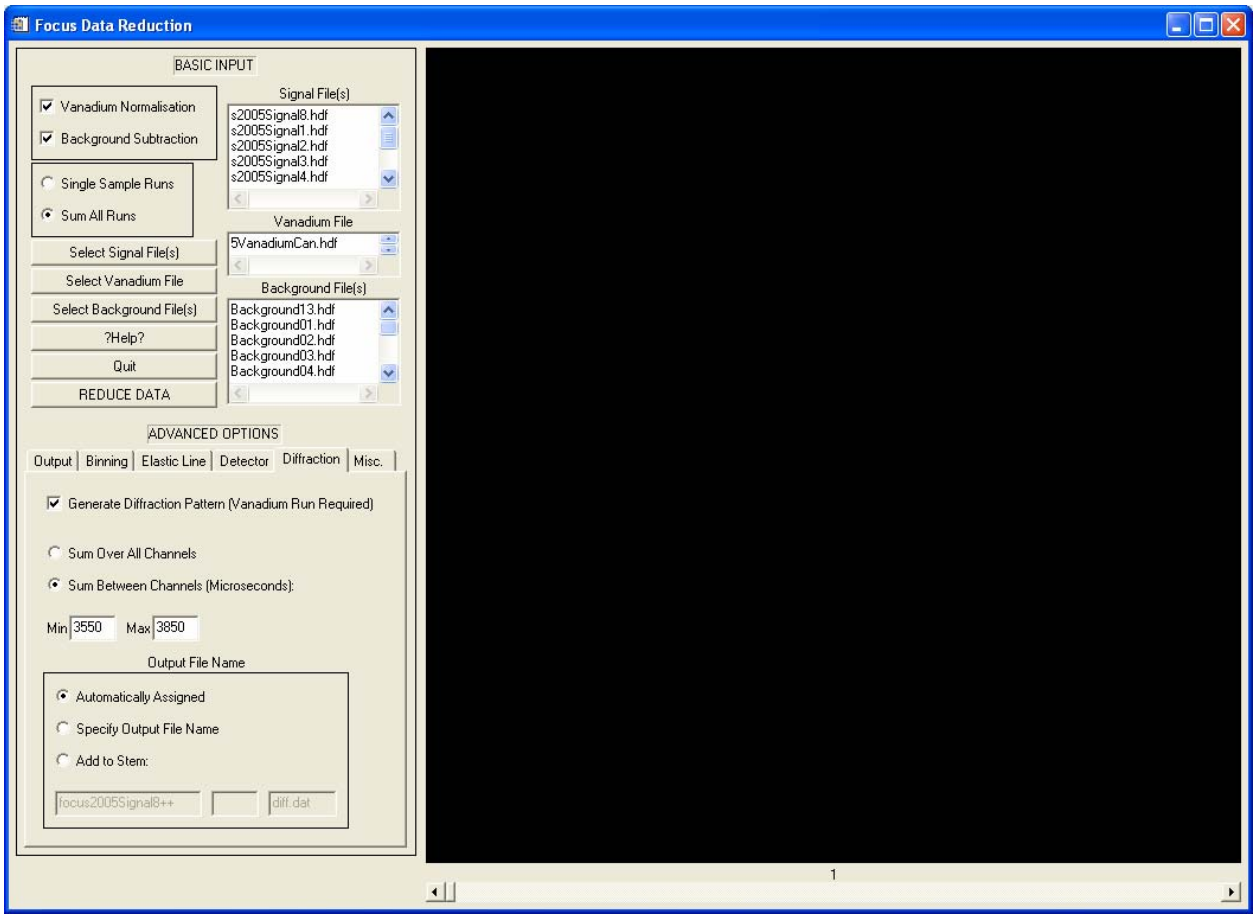
The elastic line shall be calculated from the vanadium run:



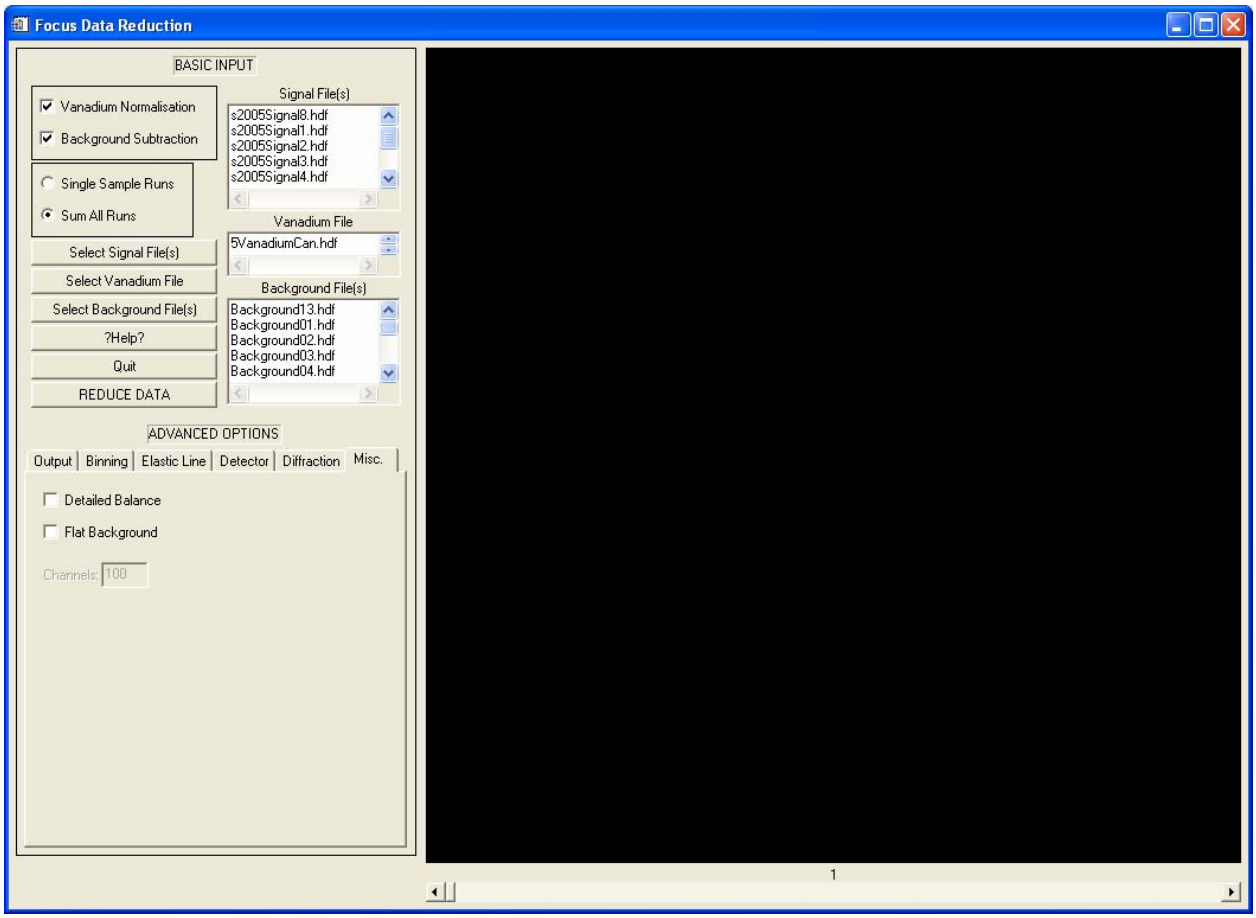
We shall incorporate detectors from all three banks, and remove the bad ones using the Graphical Masking Utility:



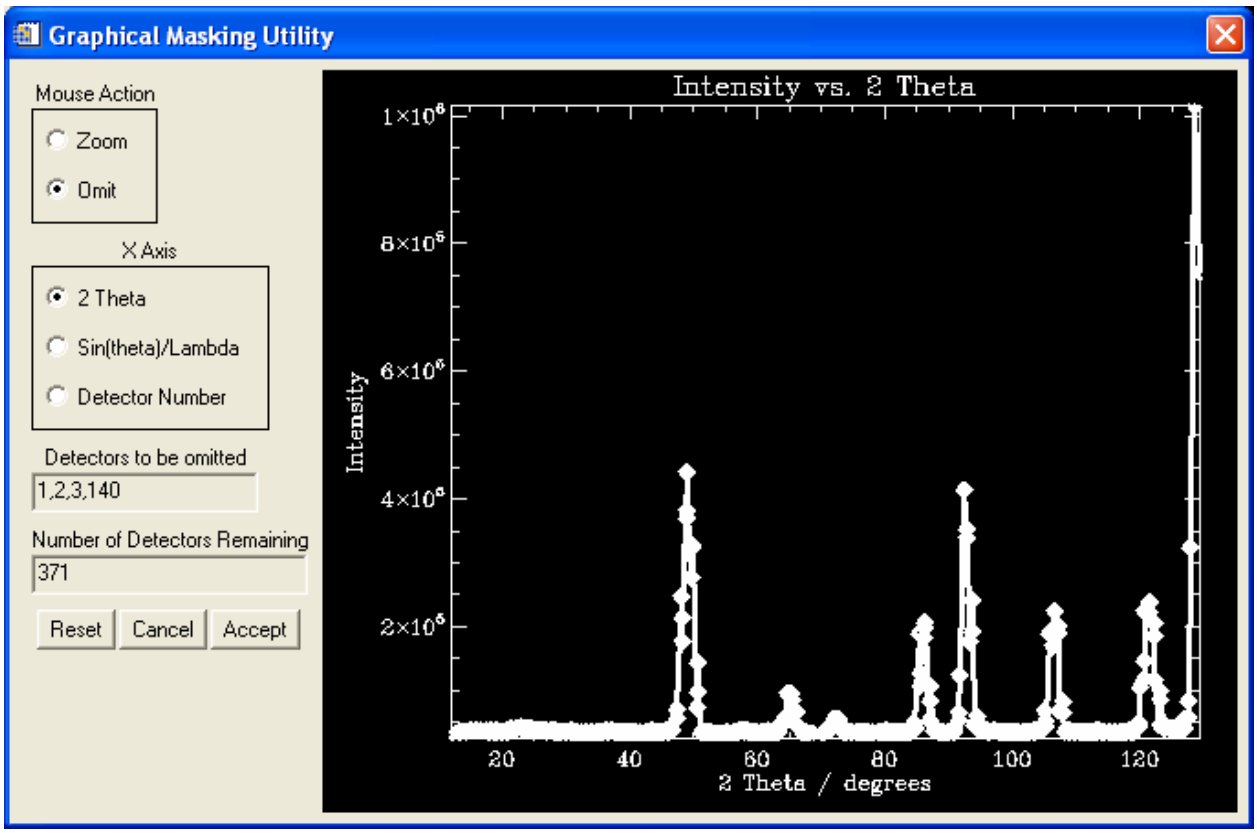
We also wish to calculate the diffraction pattern. The elastic line falls in the time window 3550 to 3850 microseconds, and we specify this time window accordingly.



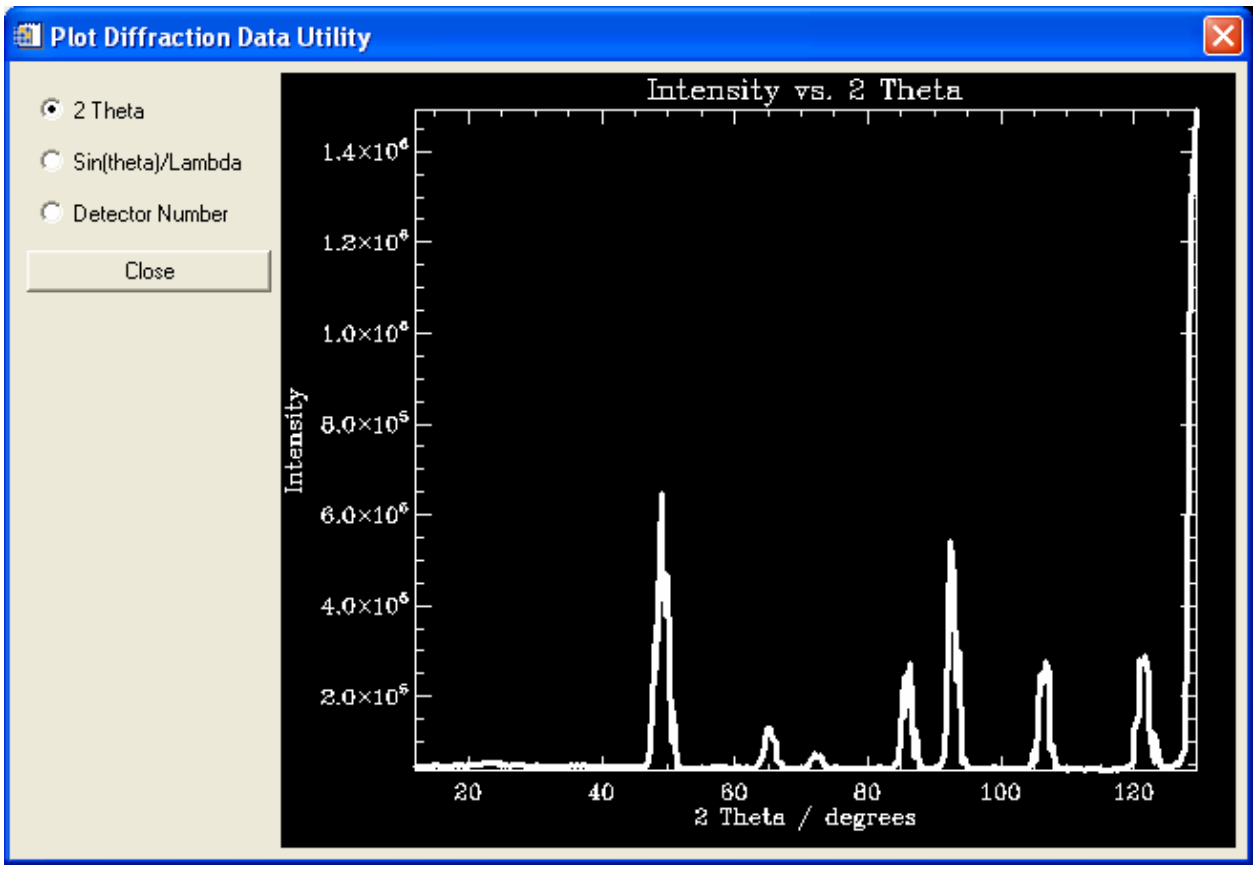
Neither the detailed balance nor the flat background option is selected. Note that if background files are selected and the flat baseline option is checked, background subtraction will proceed via subtraction of the empty can spectra only.



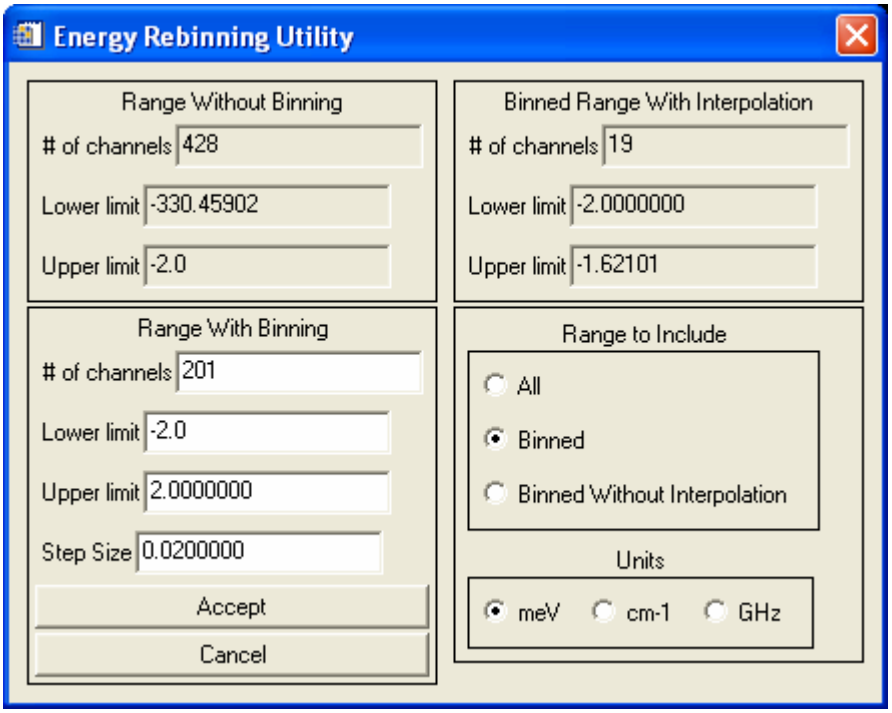
When the "REDUCE DATA" button is depressed, we are first invited to remove the bad detectors using the Graphical Masking Utility. From the screen shown below, the reader will note that detectors 1,2,3 and 140 have been removed. Detector 140 is a dead detector. If this detector is not removed at this stage, the program will crash.



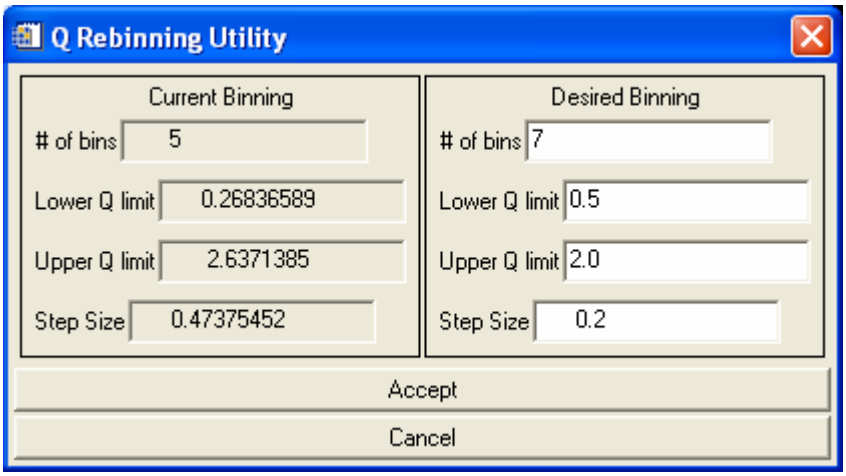
The program then reduces the detectors to a set with unique values of 2 theta. The diffraction pattern is calculated, which the user is invited to inspect:



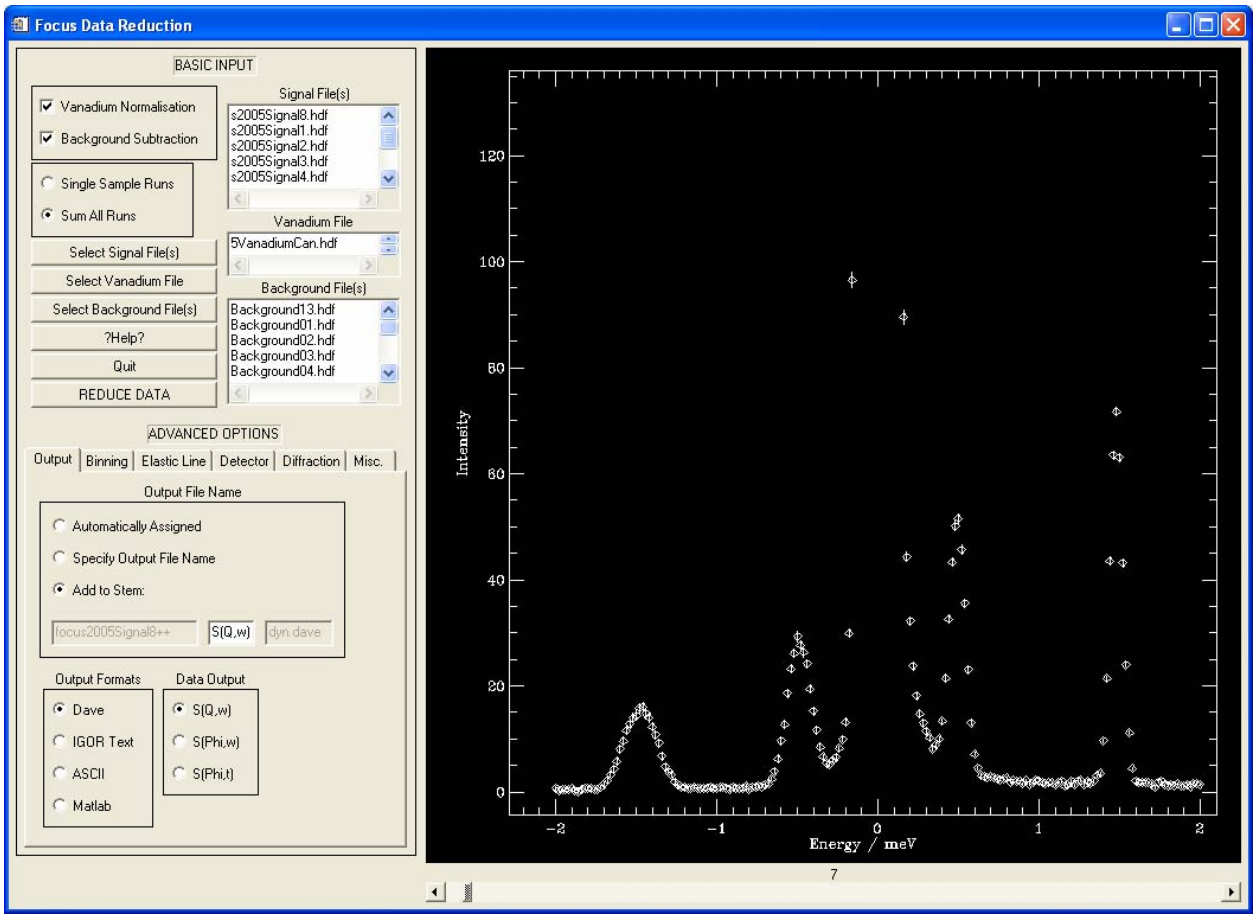
All data files are then converted to energy, and the spectra of the empty can subtracted. At this point, the user must specify the energy binning. The energy binning screen below shows that we have specified the units to be meV, with a step size of 0.02 in the range -2.0 to +2.0. The program tells us that in the binning process, points will be created in the energy range -2.0 to -1.62 meV.



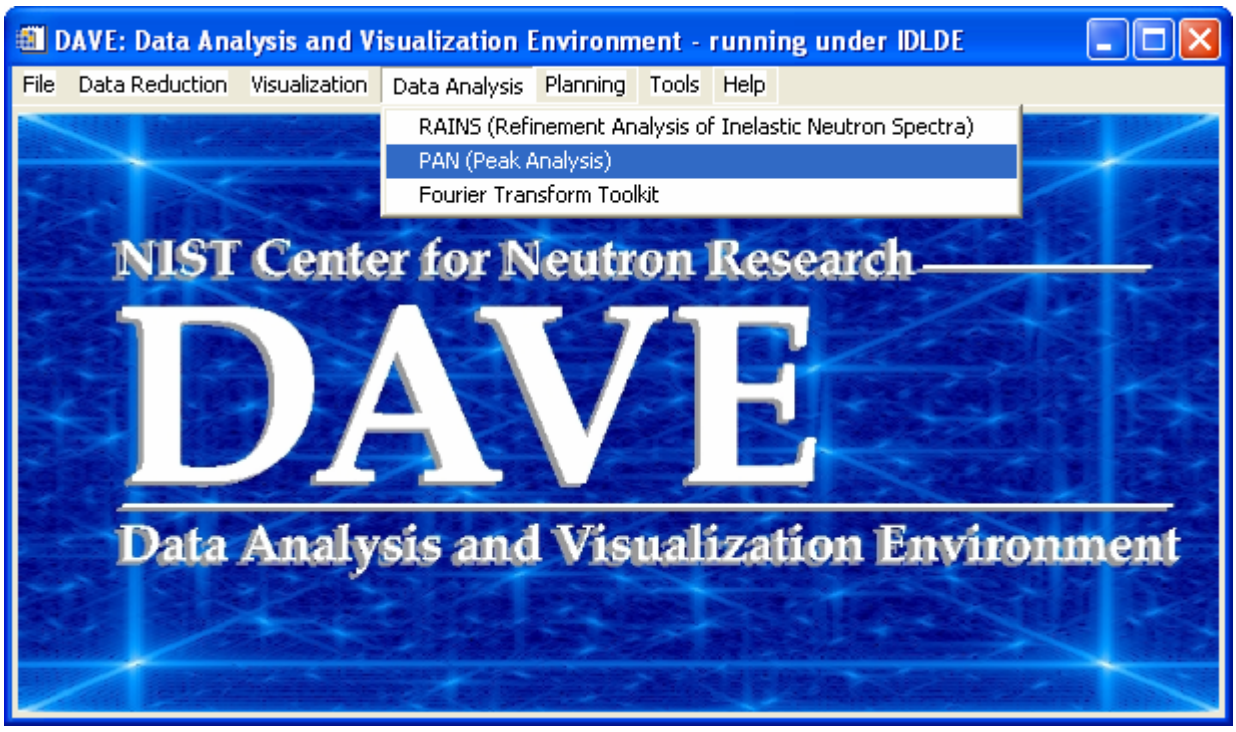
On pressing the "Accept" button, the Q Rebinning Utility appears. The default Q range is the maximum possible for the specified energy window. Since, however, we are interested in examining the Q-dependence of the transition that falls between 1.0 and 2.0 meV, we must set the minimum and maximum Q value to 0.5 and 2.0 $Å^{-1}$ respectively, as previously determined by the neutron calculator. We specify a step size of 0.2 $Å^{-1}$, resulting in 7 Q bins.



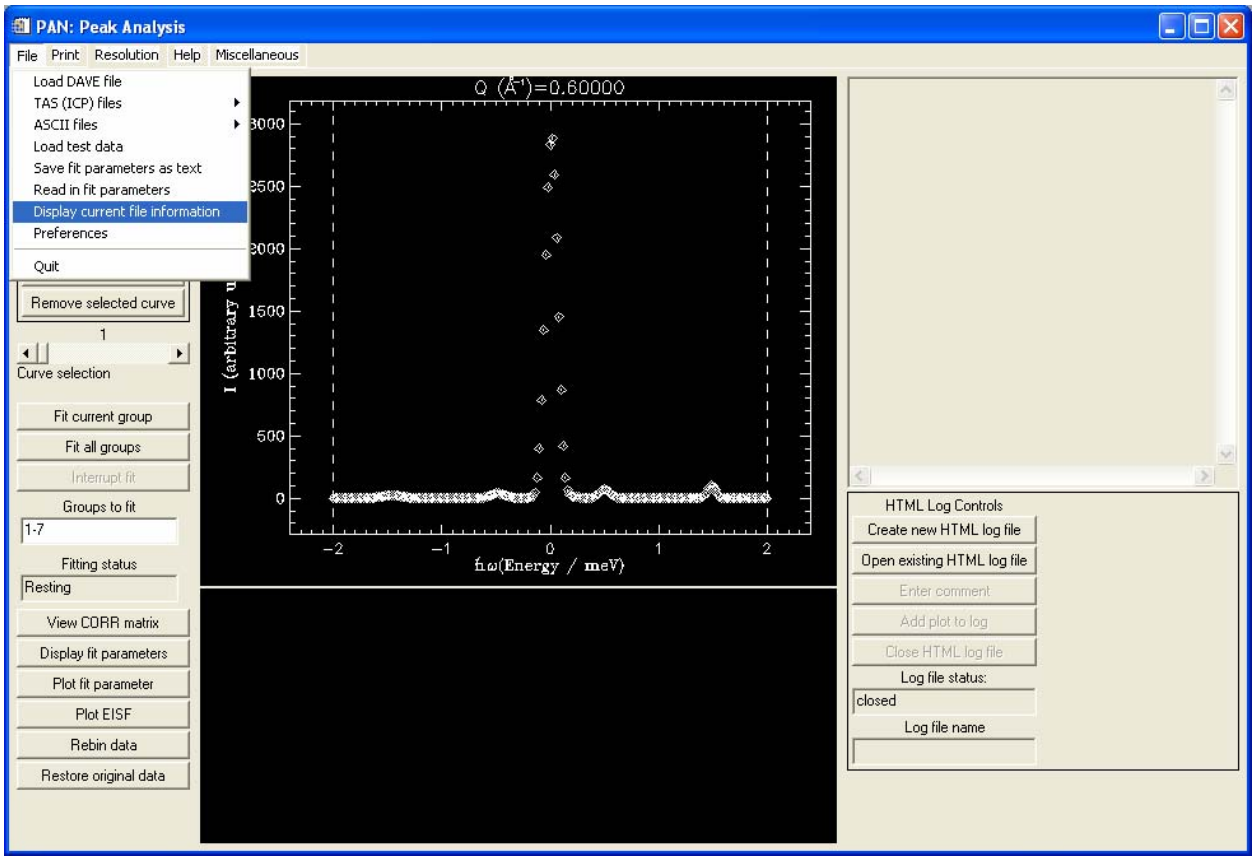
The data are then reduced. Seven spectra are calculated in total, corresponding to the seven Q bins. At this stage we are able to zoom in on the portion of the spectrum of interest, and view each spectrum utilising the group slider.

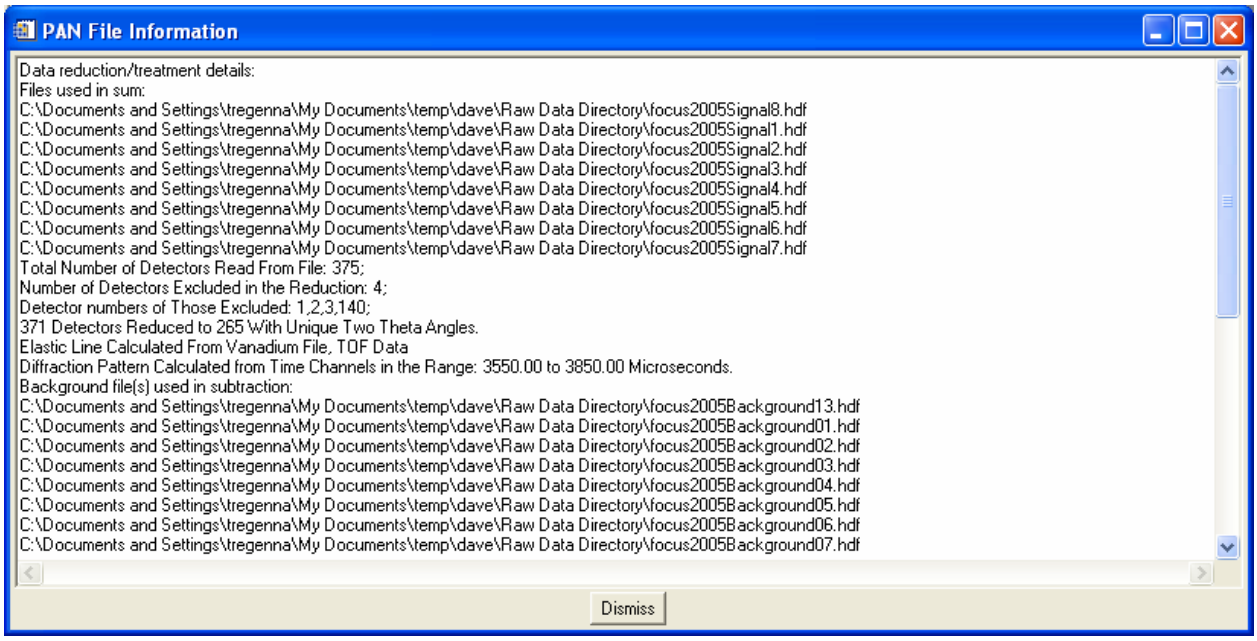


We have now done all we can with FDR. The data analysis program, PAN, is then initialised after quitting FDR.

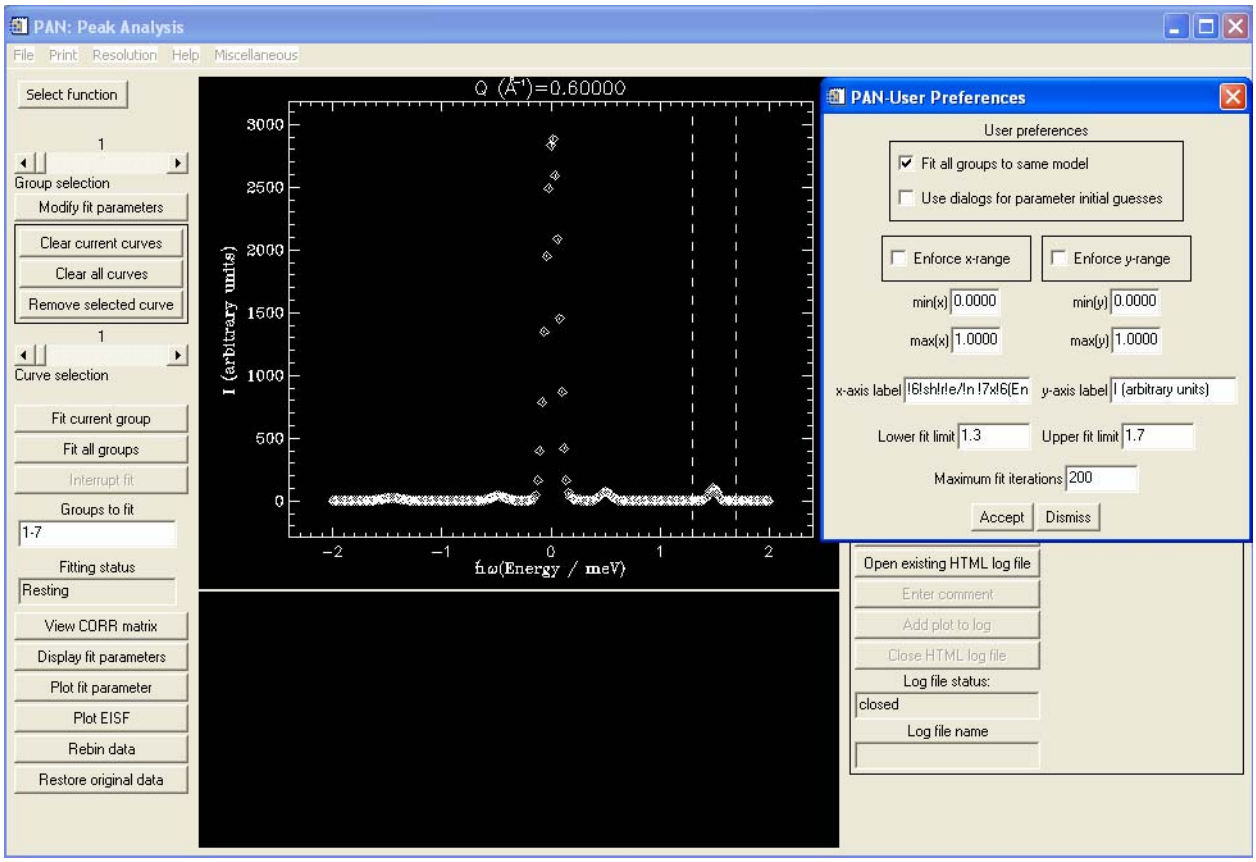


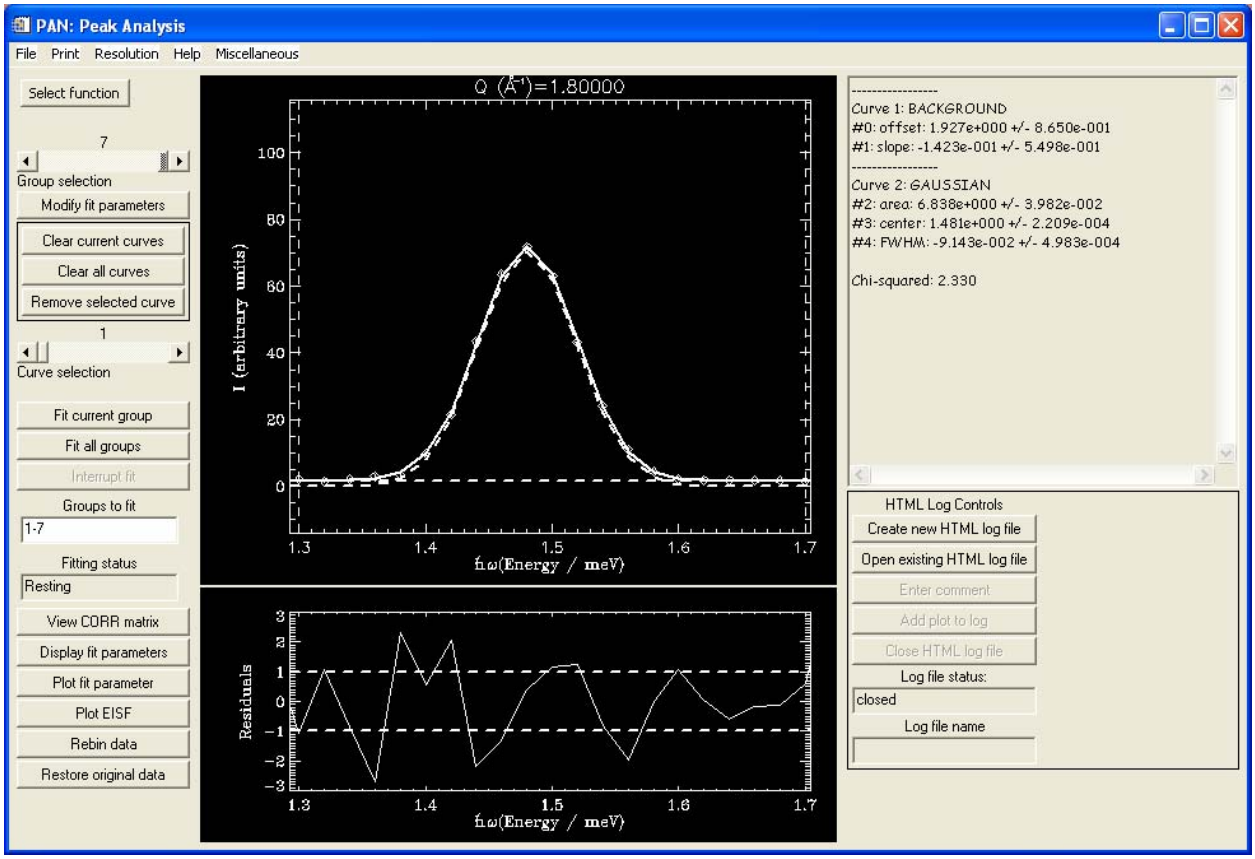
The data just reduced are read in automatically by PAN. The details of the reduction process just undertaken may be viewed by selecting "Display Current File Information":

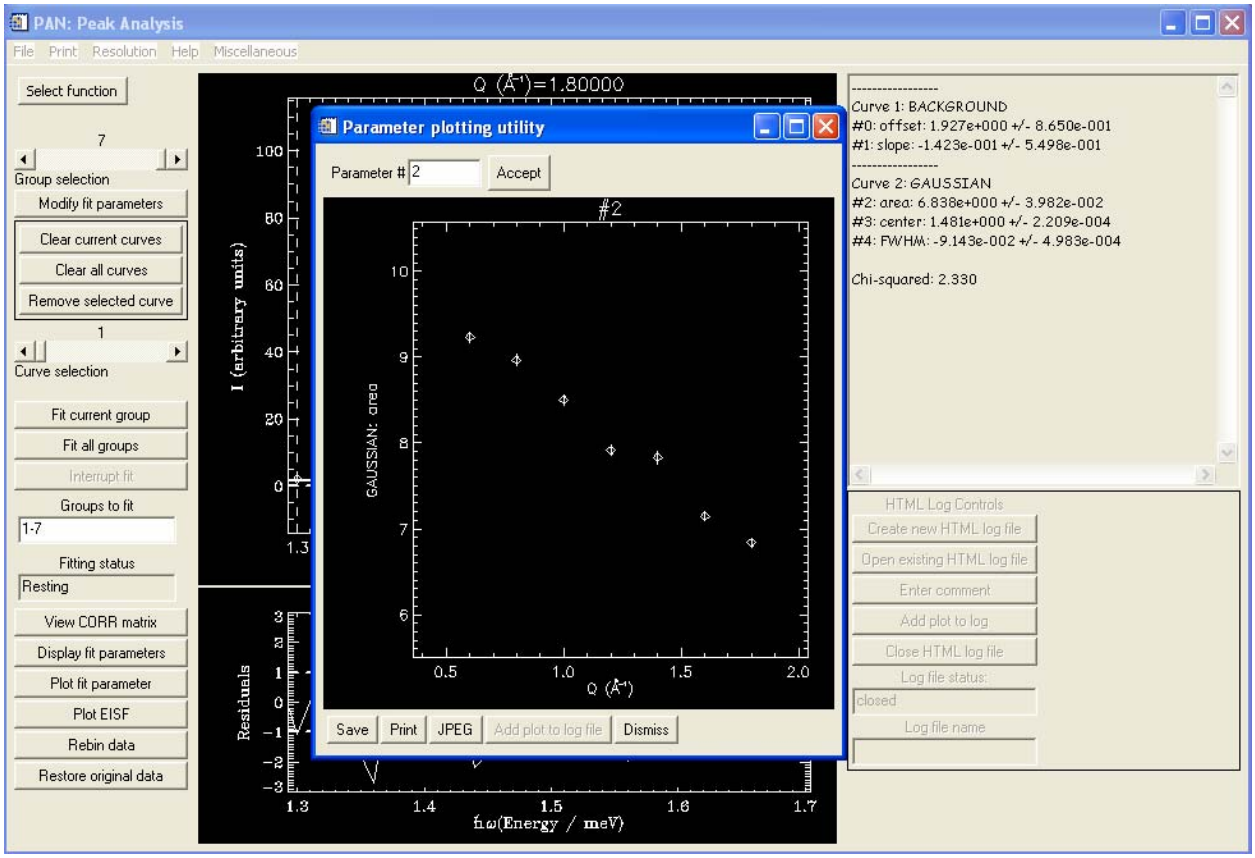




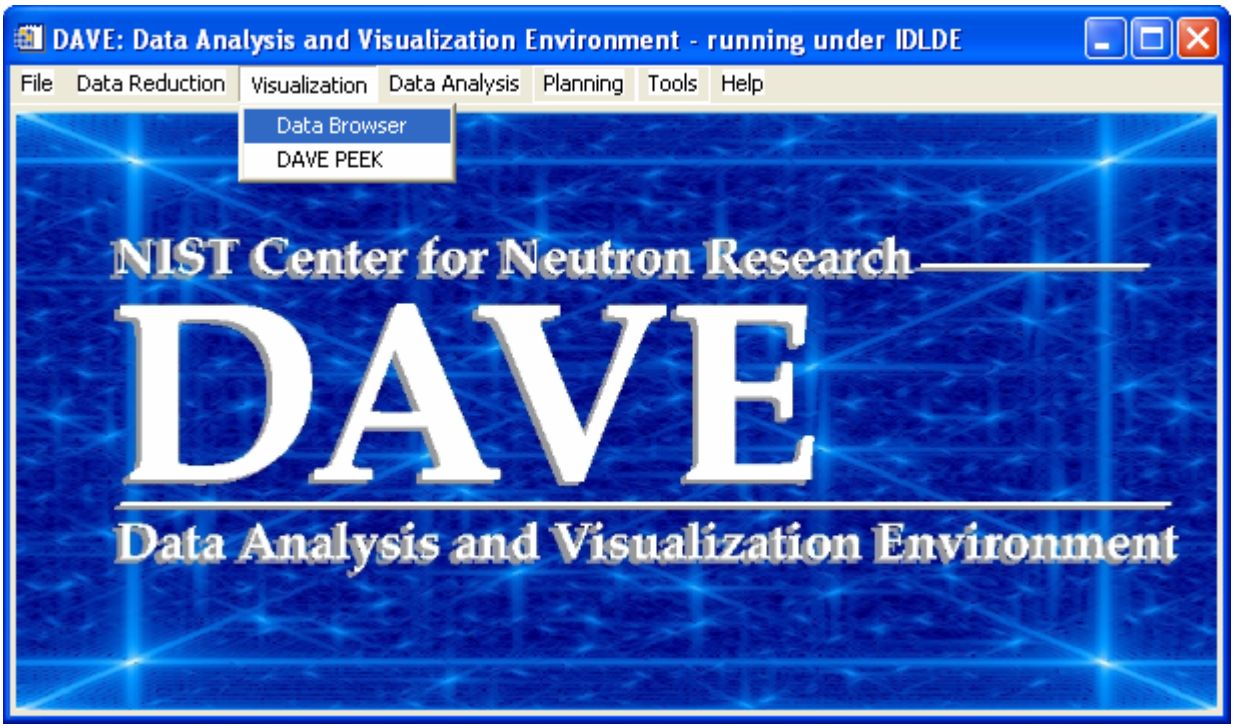
PAN may be used to model the spectra as a superposition of different functions. In order to examine the Q-dependence of the intensity of the high-energy peak, the peak is fitted to a superposition of a linear background and Gaussian function, and the area of the Gaussian function plotted as a function of Q. The area of the peak in the seven files can be exported to an ascii file as shown. Please consult the PAN help file for futher details.

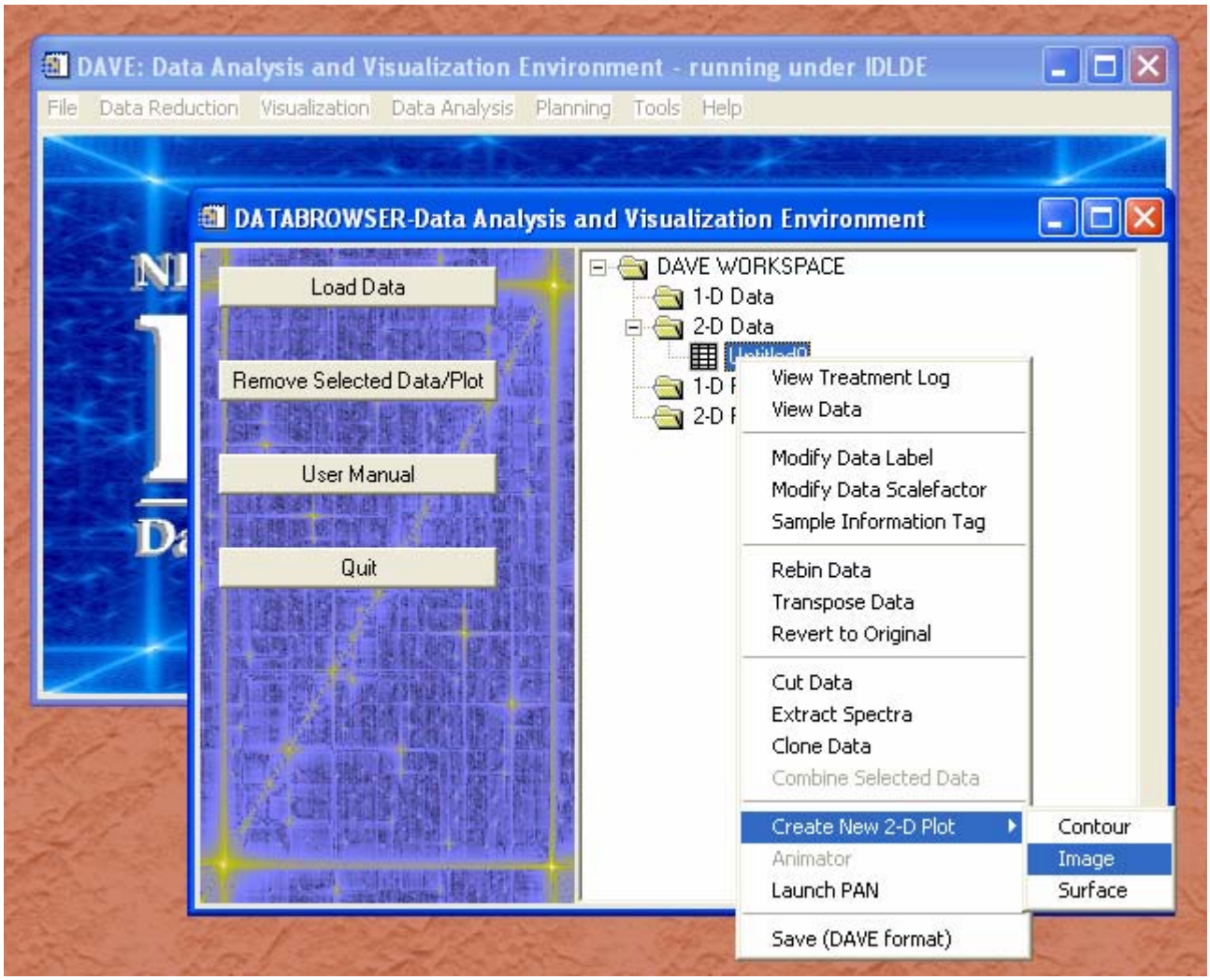

PAN: Peak Analysis
File Print Resolution Help Miscellaneous
Select function
Group selection
Modify fit parameters
Clear current curves
Clear all curves
Remove selected curve
Curve selection
Fit current group
Fit all groups
Interrupt fit
Groups to fit
1-7
Fitting status
Resting
View CORR matrix
Display fit parameters
Plot fit parameter
Plot EISF
Rebin data
Restore original data
Q (Å⁻¹)=0.60000
I (arbitrary units)
ħω(Energy / meV)
PAN-User Preferences
User preferences
Fit all groups to same model
Use dialogs for parameter initial guesses
Enforce x-range
Enforce y-range
min(x) 0.0000
min(y) 0.0000
max(x) 1.0000
max(y) 1.0000
x-axis label
y-axis label I (arbitrary units)
Lower fit limit 1.3
Upper fit limit 1.7
Maximum fit iterations 200
Accept
Dismiss
Open existing HTML log file
Enter comment
Add plot to log
Close HTML log file
Log file status:
closed
Log file name

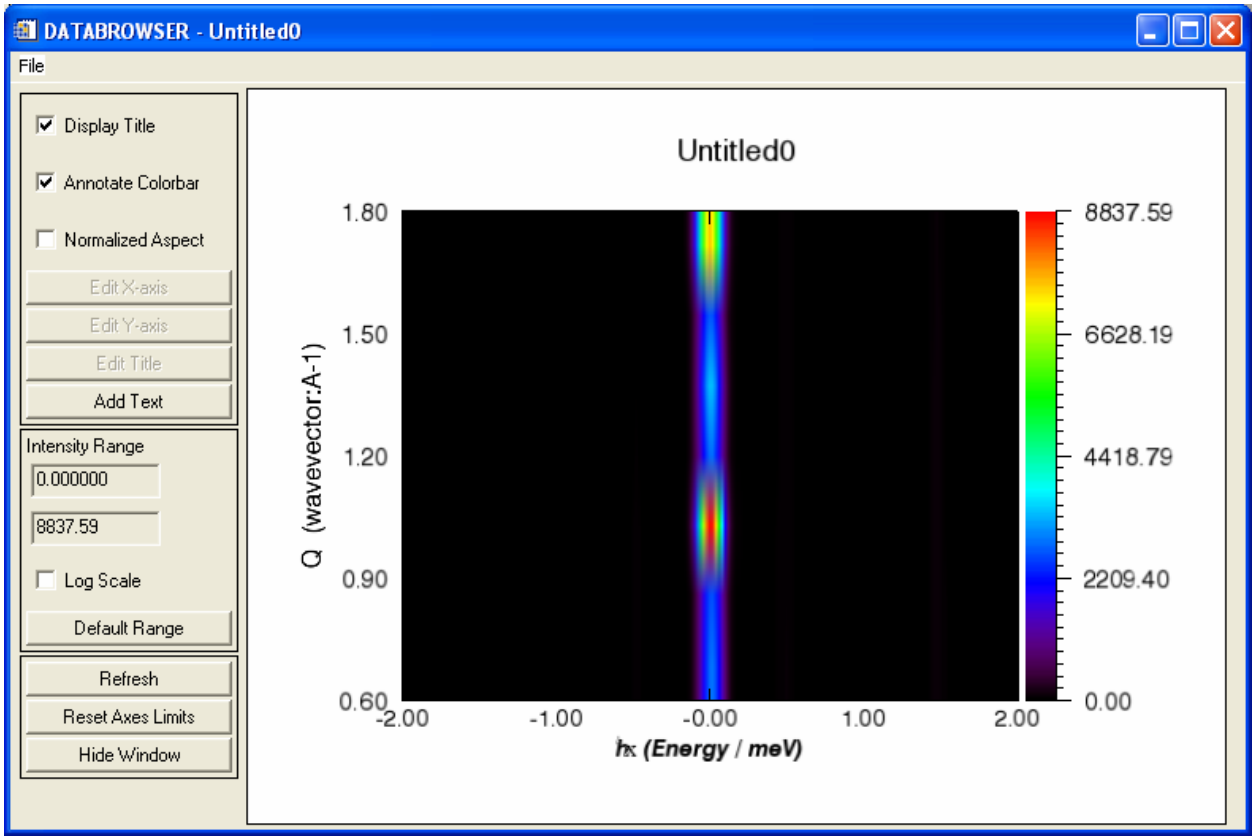

PAN: Peak Analysis
File
Print
Resolution
Help
Miscellaneous
Select function
7
Group selection
Modify fit parameters
Clear current curves
Clear all curves
Remove selected curve
1
Curve selection
Fit current group
Fit all groups
Interrupt fit
Groups to fit
1-7
Fitting status
Resting
View CORR matrix
Display fit parameters
Plot fit parameter
Plot EISF
Rebin data
Restore original data
Q (Å⁻¹)=1.80000
I (arbitrary units)
ħω(Energy / meV)
Residuals
ħω(Energy / meV)
Curve 1: BACKGROUND
#0: offset: 1.927e+000 +/- 8.650e-001
#1: slope: -1.423e-001 +/- 5.498e-001
Curve 2: GAUSSIAN
#2: area: 6.838e+000 +/- 3.982e-002
#3: center: 1.481e+000 +/- 2.209e-004
#4: FWHM: -9.143e-002 +/- 4.983e-004
Chi-squared: 2.330
HTML Log Controls
Create new HTML log file
Open existing HTML log file
Enter comment
Add plot to log
Close HTML log file
Log file status:
closed
Log file name

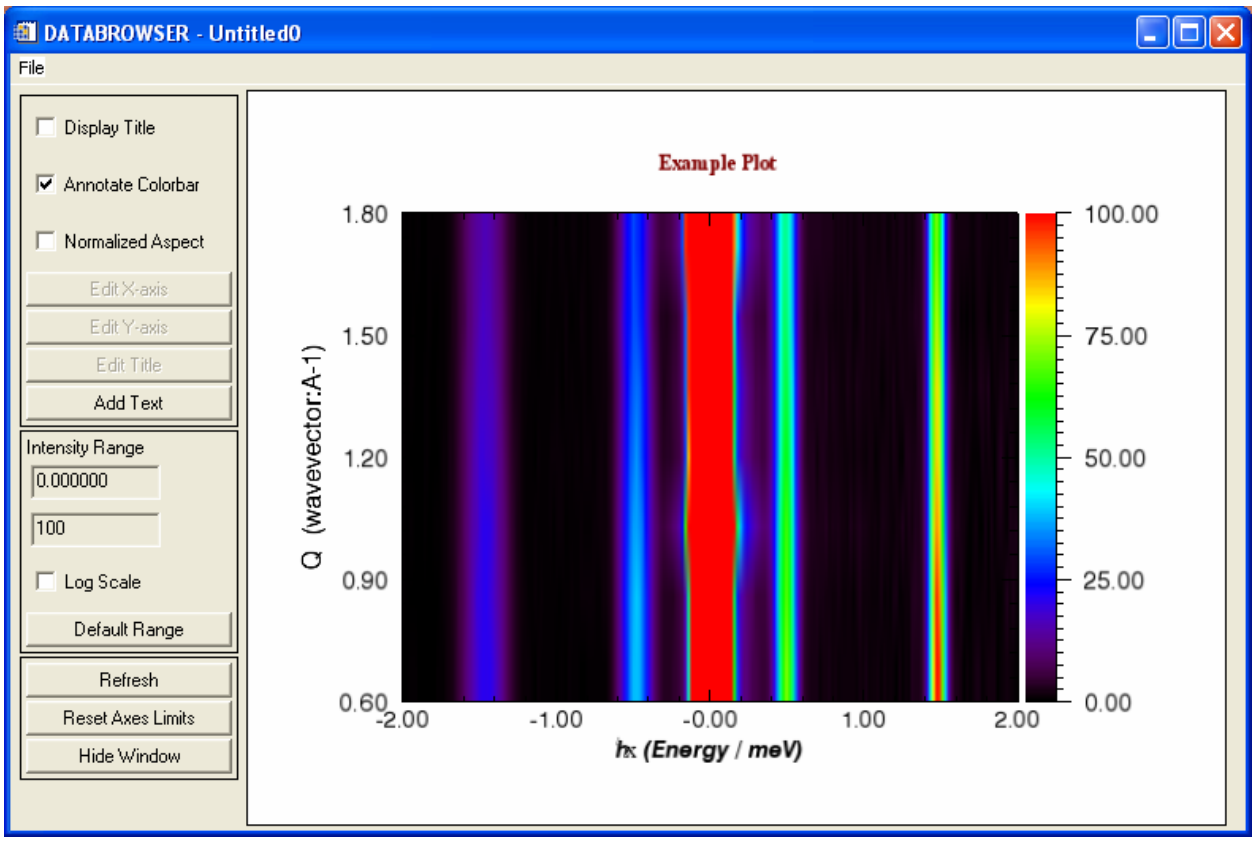


The data may be displayed using the data browser program program, which is found under visualization.




DAVE: Data Analysis and Visualization Environment - running under IDLDE
File
Data Reduction
Visualization
Data Analysis
Planning
Tools
Help
DATABROWSER-Data Analysis and Visualization Environment
Load Data
Remove Selected Data/Plot
User Manual
Quit
DAVE WORKSPACE
1-D Data
2-D Data
View Treatment Log
View Data
Modify Data Label
Modify Data Scalefactor
Sample Information Tag
Rebin Data
Transpose Data
Revert to Original
Cut Data
Extract Spectra
Clone Data
Combine Selected Data
Create New 2-D Plot
Animator
Launch PAN
Save (DAVE format)
Contour
Image
Surface


DATABROWSER - Untitled0
File
Display Title
Annotate Colorbar
Normalized Aspect
Edit X-axis
Edit Y-axis
Edit Title
Add Text
Intensity Range
0.000000
8837.59
Log Scale
Default Range
Refresh
Reset Axes Limits
Hide Window
Untitled0
1.80
1.50
1.20
0.90
0.60
Q (wavevector:A-1)
-2.00
-1.00
-0.00
1.00
2.00
ħω (Energy / meV)
8837.59
6628.19
4418.79
2209.40
0.00


DATABROWSER - Untitled0
File
Display Title
Annotate Colorbar
Normalized Aspect
Edit X-axis
Edit Y-axis
Edit Title
Add Text
Intensity Range
0.000000
100
Log Scale
Default Range
Refresh
Reset Axes Limits
Hide Window
Example Plot
1.80
1.50
1.20
0.90
0.60
Q (wavevector:A-1)
-2.00
-1.00
-0.00
1.00
2.00
ħω (Energy / meV)
100.00
75.00
50.00
25.00
0.00