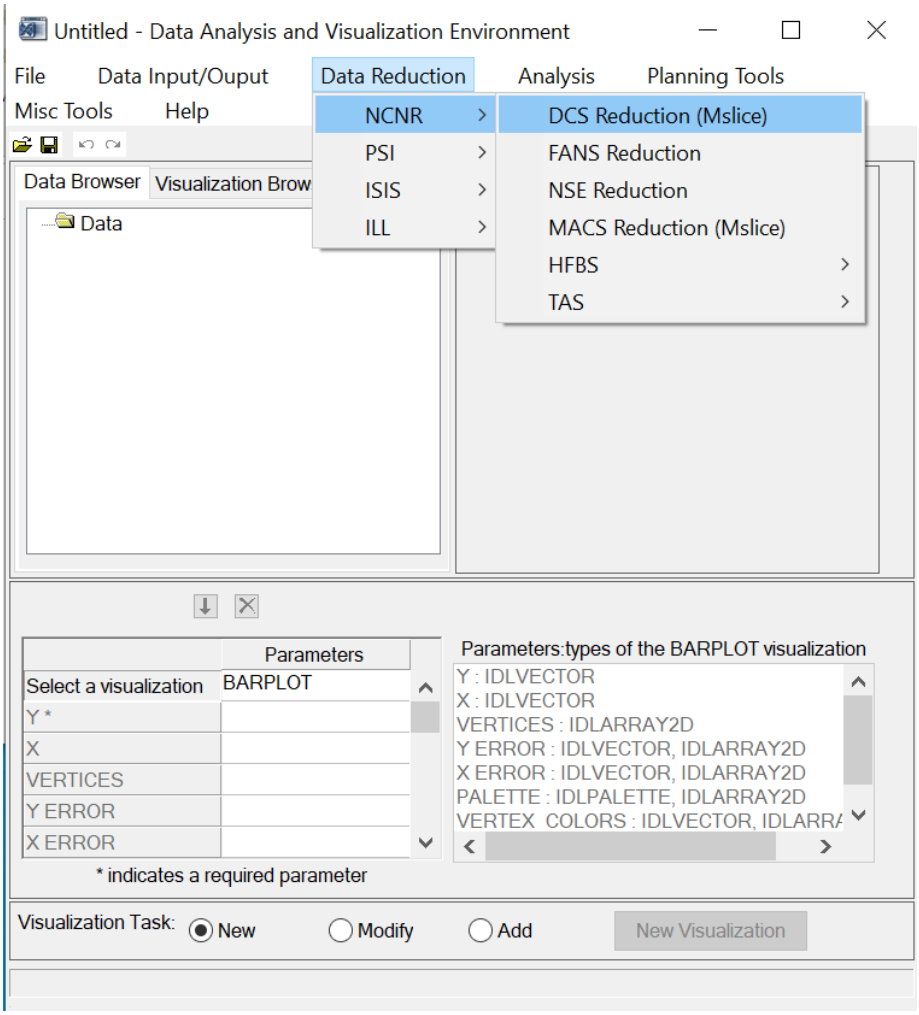
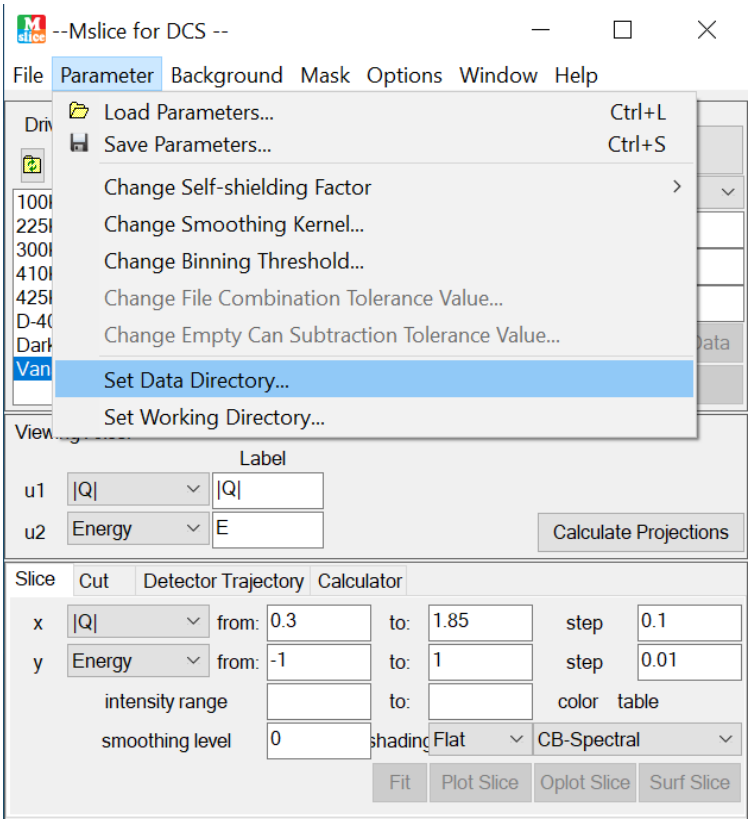
DCS data reduction and analysis: a quick manual

In the summer school, we are doing QENS experiments on powder samples using DCS. Here is a quick manual showing how we do data reduction and analysis. (Note that for DCS data on single crystal samples, the data reduction procedure would be significantly different.)

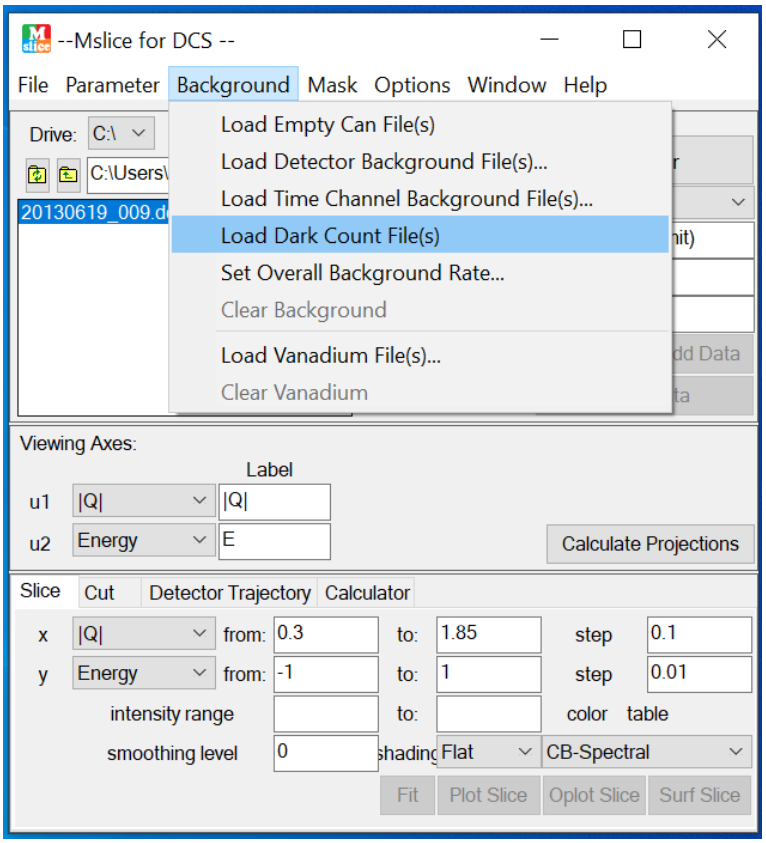
We use the program Mslice in the DAVE package for data reduction. (For detailed instructions on how to use Mslice, please refer to:
http://www.ncnr.nist.gov/dave/documentation/dcs_mslice.pdf)



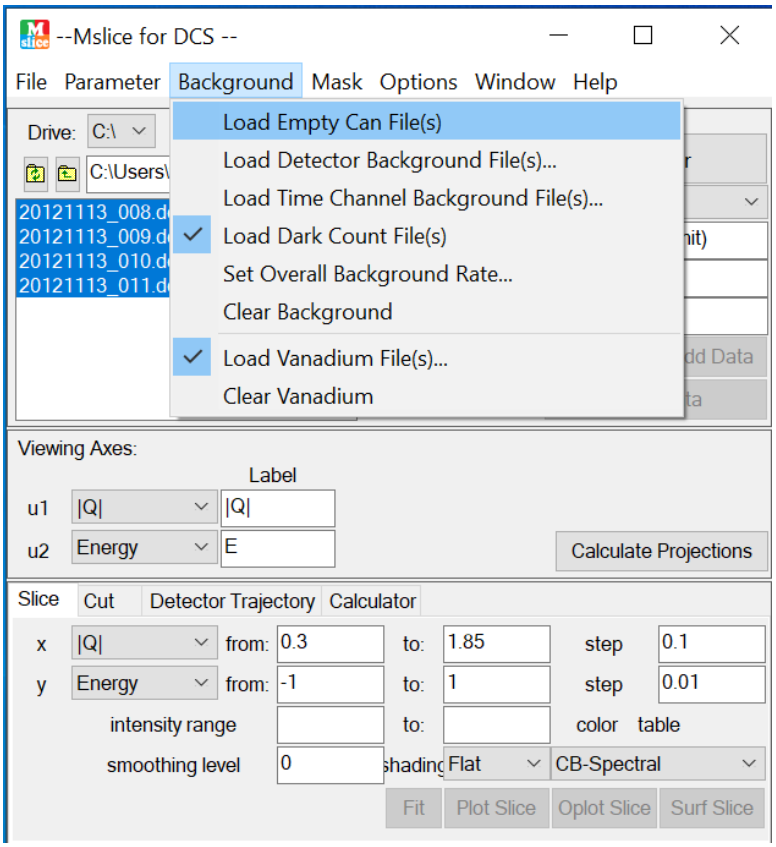
In Mslice, we can set the Data Directory and Working Directory, just for convenience.



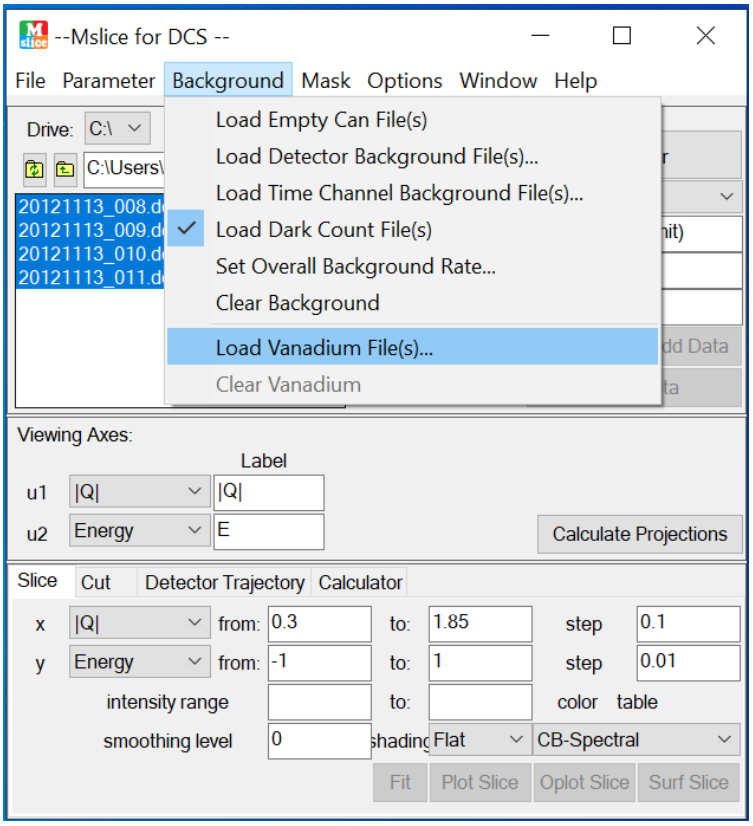
For the program to take care of background subtraction during data reduction, highlight the corresponding files and load them. Shown below is the “dark count” (beam closed) background subtraction.



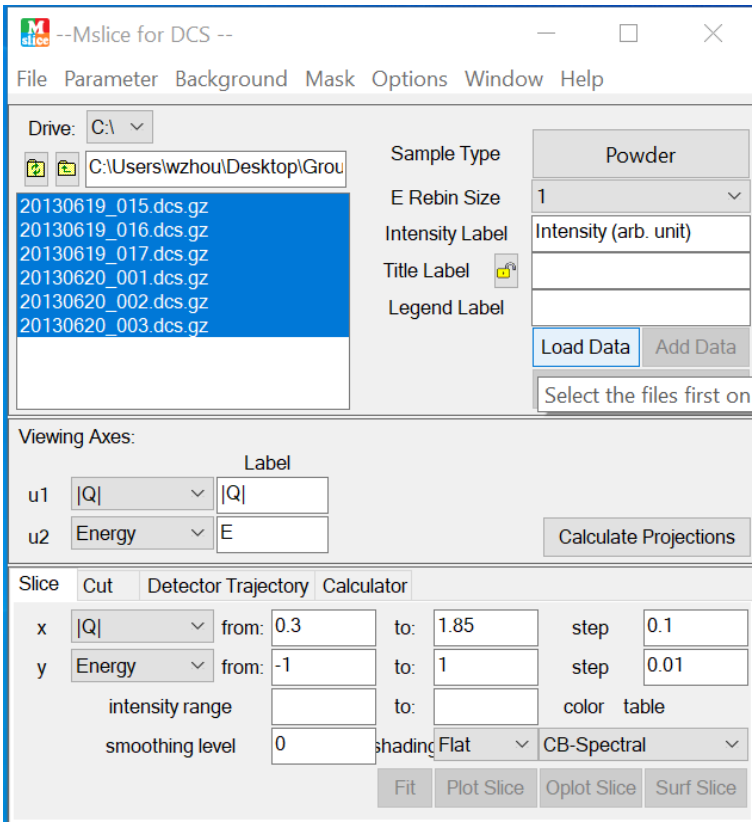
If we have data measured for the empty can, we can do empty can background subtraction, in which case we would not need the “dark count” background subtraction (the empty can data would already include dark count fast background).

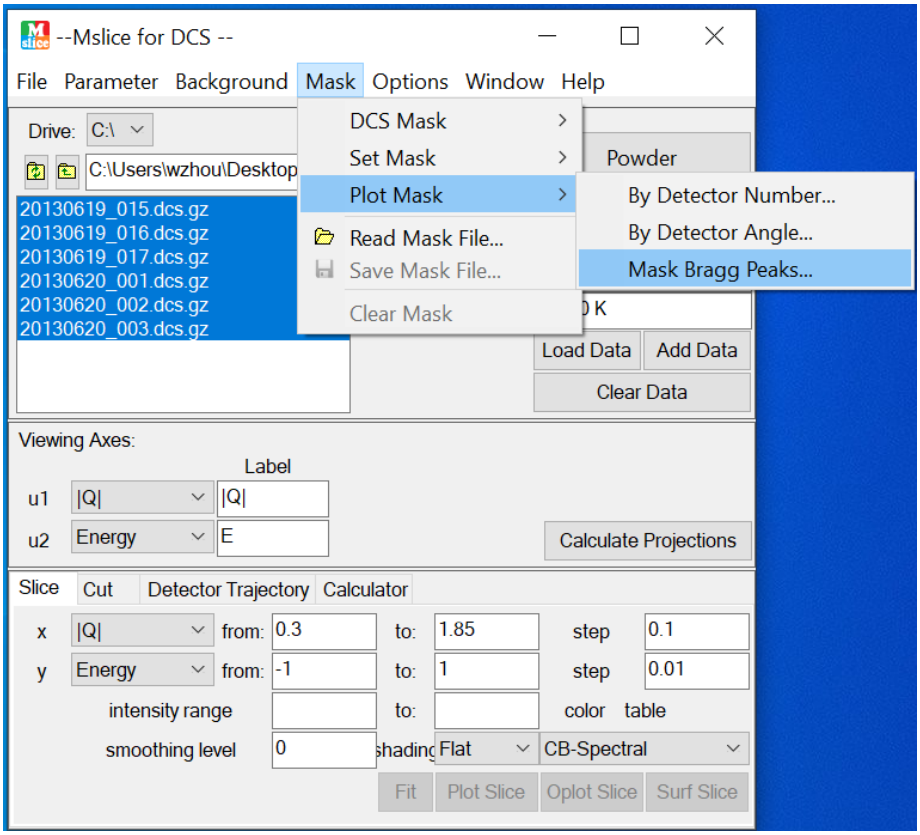


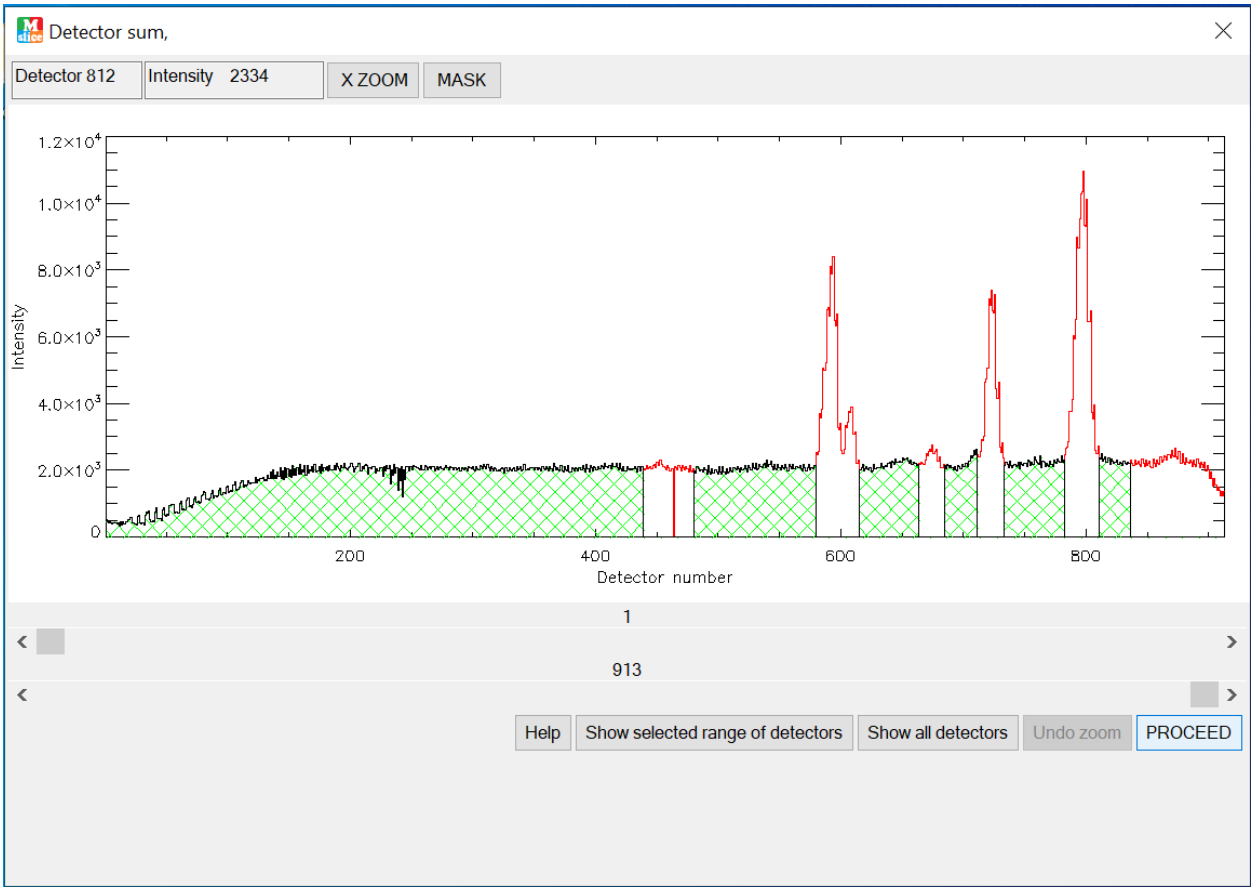
To correct detector efficiencies, we load the vanadium files.



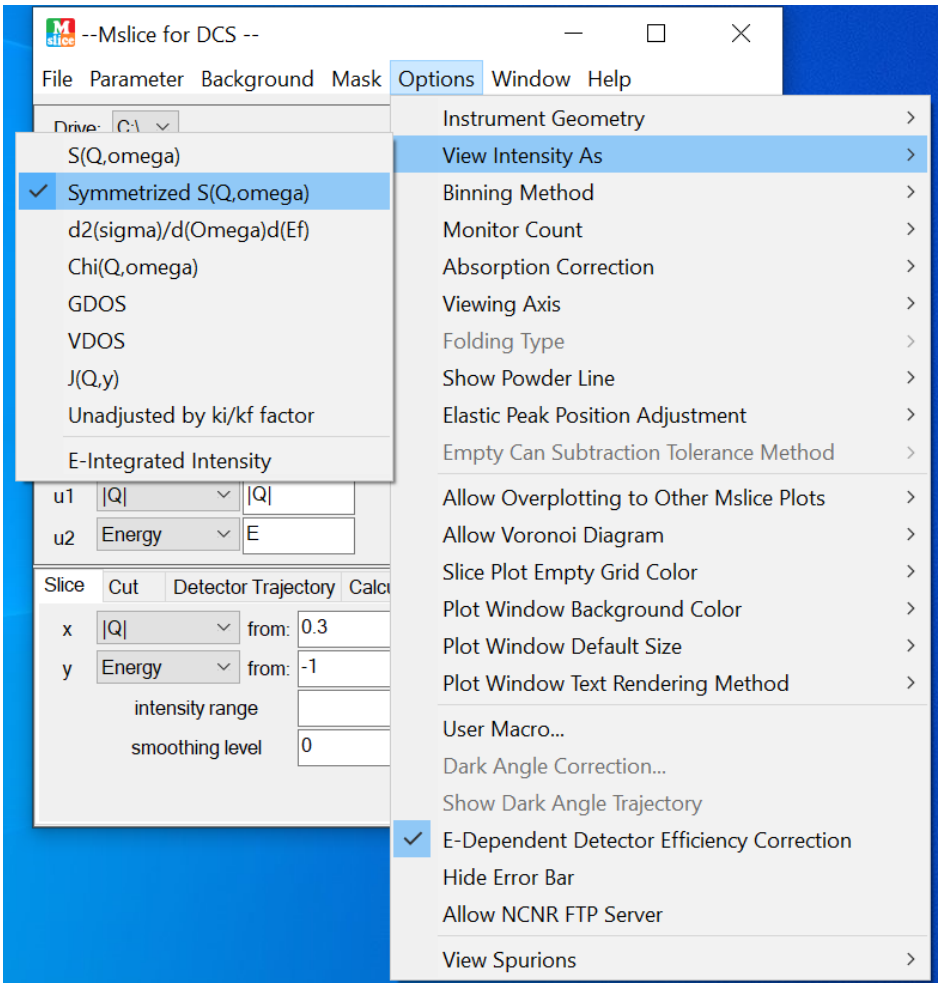
For QENS analysis, to omit detectors that contain Bragg peak intensity, we load the sample data first, and then “Mask Bragg Peaks”.



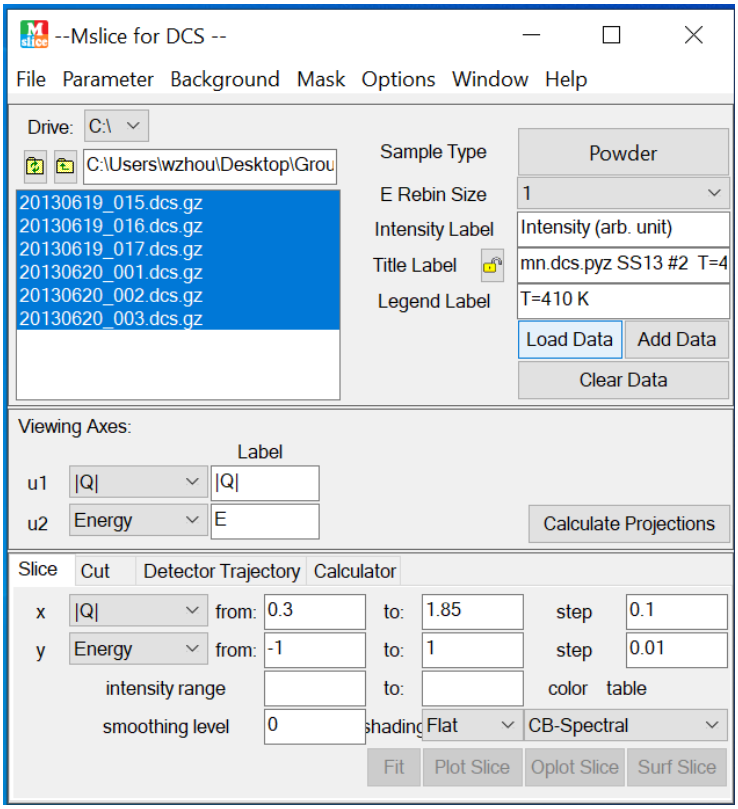

--Mslice for DCS --
File Parameter Background Mask Options Window Help
DCS Mask
Set Mask
Plot Mask
Read Mask File...
Save Mask File...
Clear Mask
By Detector Number...
By Detector Angle...
Mask Bragg Peaks...
Drive: C:\
C:\Users\wzhou\Desktop
Powder
20130619_015.dcs.gz
20130619_016.dcs.gz
20130619_017.dcs.gz
20130620_001.dcs.gz
20130620_002.dcs.gz
20130620_003.dcs.gz
Load Data
Add Data
Clear Data
Viewing Axes:
Label
u1 |Q| |Q|
u2 Energy E
Calculate Projections
Slice Cut Detector Trajectory Calculator
x |Q| from: 0.3 to: 1.85 step 0.1
y Energy from: -1 to: 1 step 0.01
intensity range to: color table
smoothing level 0 shading Flat CB-Spectral
Fit Plot Slice Oplot Slice Surf Slice

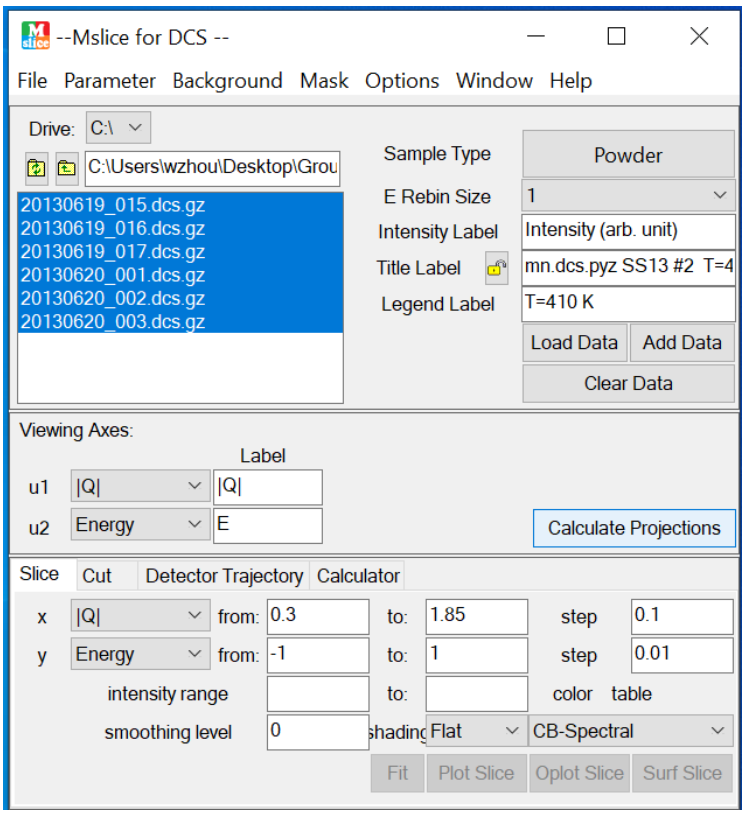

Detector sum,
Detector 812
Intensity 2334
X ZOOM
MASK
1.2×10^4
1.0×10^4
8.0×10^3
6.0×10^3
4.0×10^3
2.0×10^3
0
Intensity
200
400
600
800
Detector number
1
913
Help
Show selected range of detectors
Show all detectors
Undo zoom
PROCEED

For QENS analysis, the symmetrized S(Q, ω) is what we want, so we change the “View Intensity As” selection accordingly.

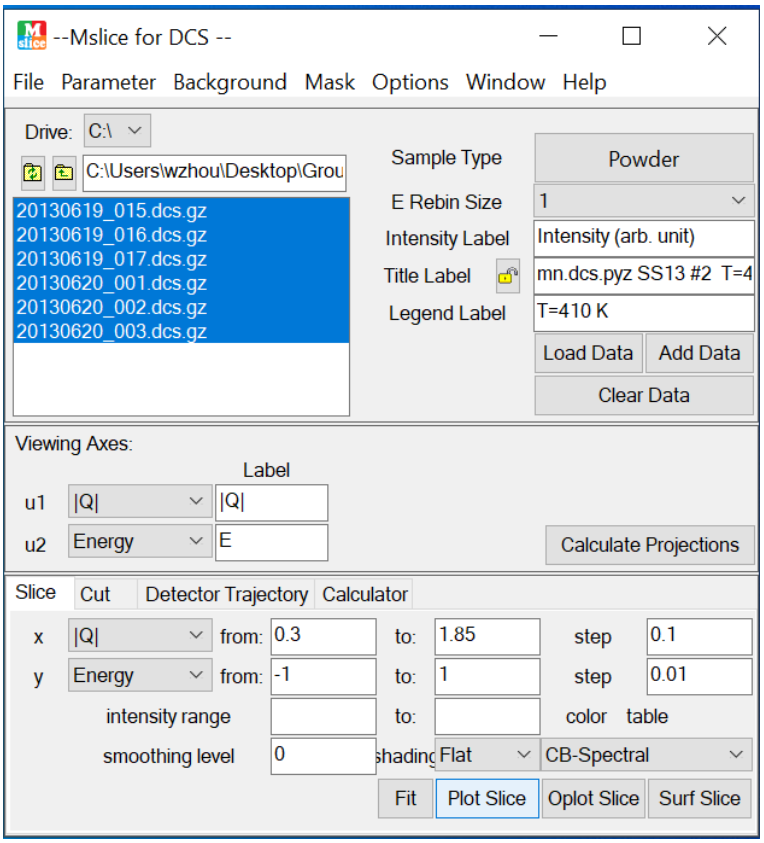


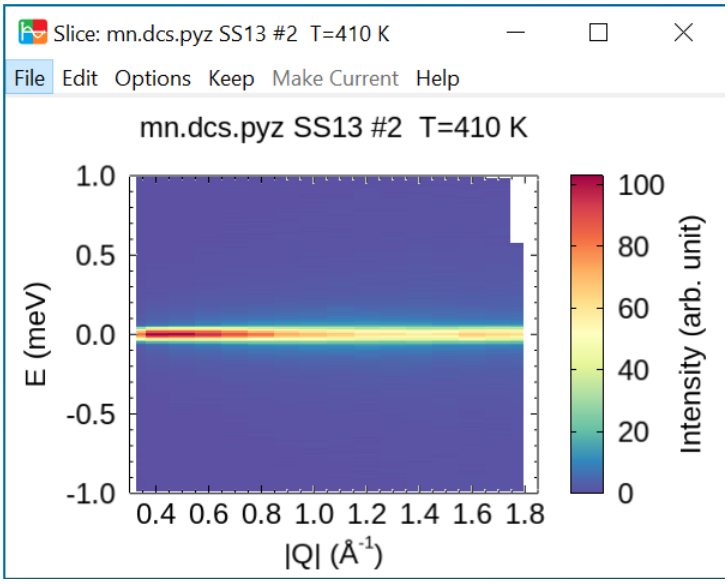
Now we can reload the data and click “Calculate Projections”.



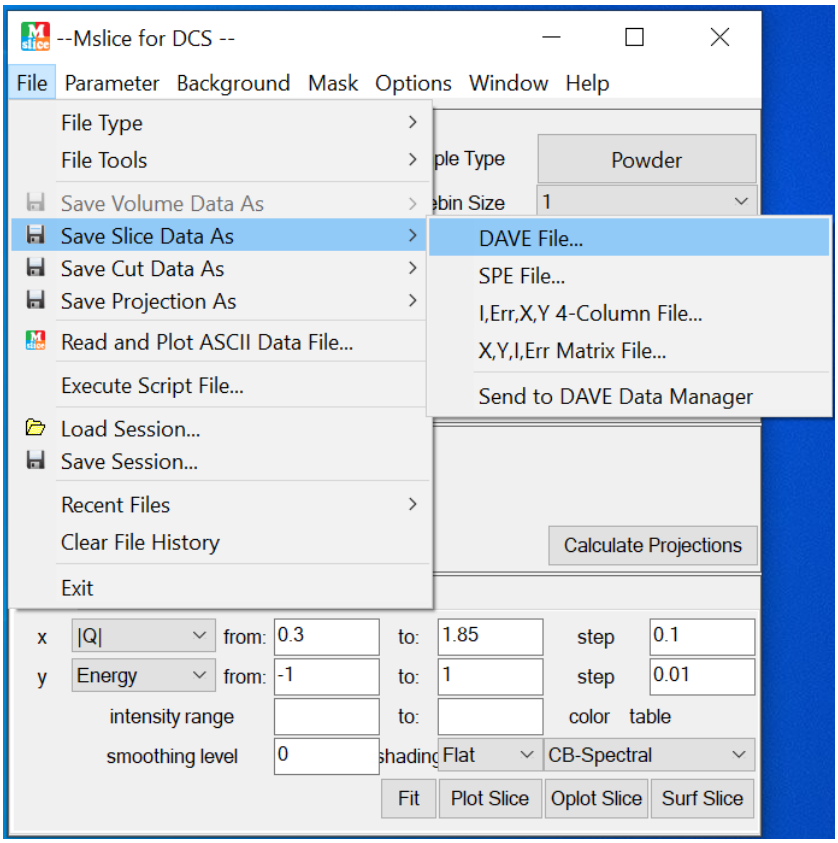


Now we are ready to plot the data. We can use “Plot Slice” to plot the Intensity as function of both Q and E.

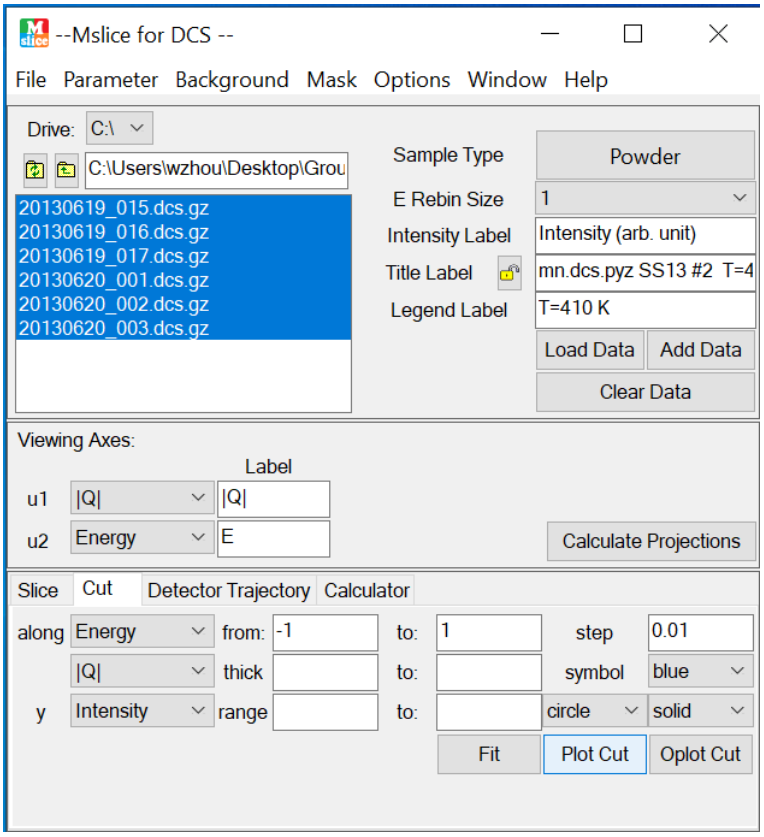


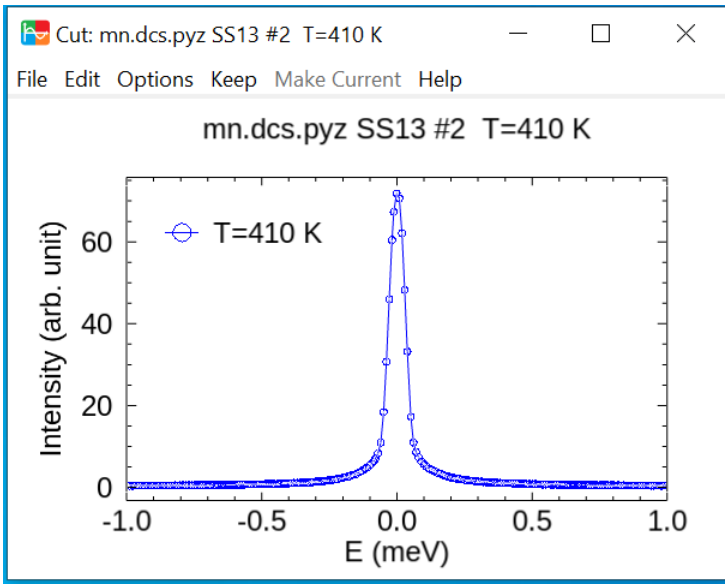


The Slice data can be saved as a DAVE file (to be analyzed using the PAN program) or in some other ASCII format.

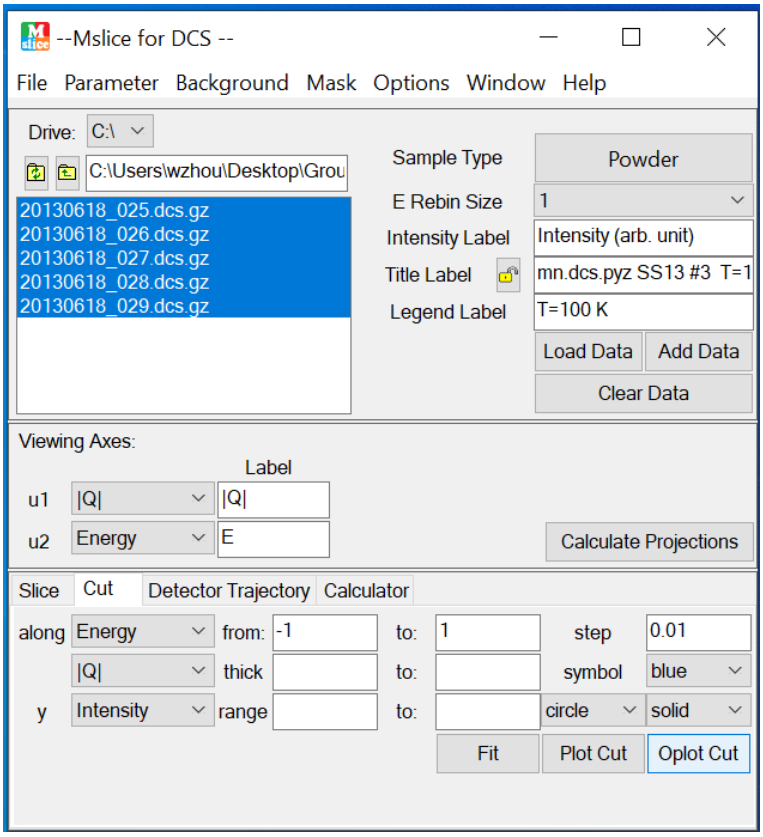


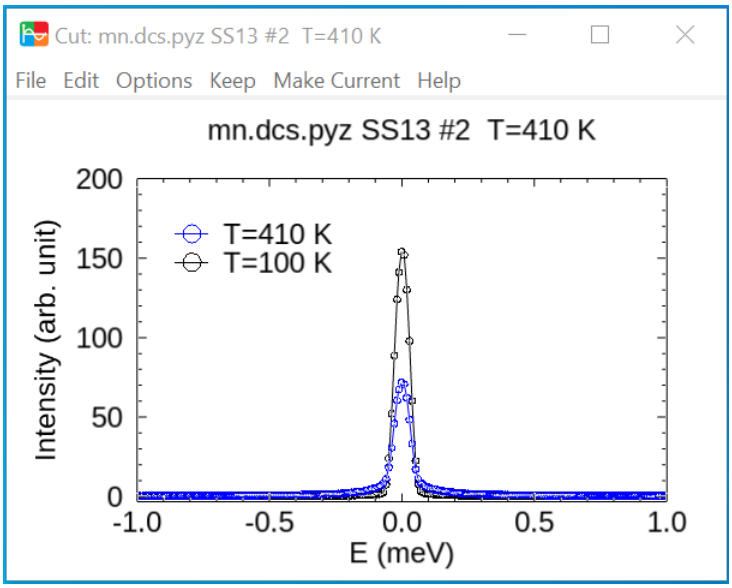
The data can also be plotted as “Cut” (e.g., Intensity vs. Q or Intensity vs. E etc.)



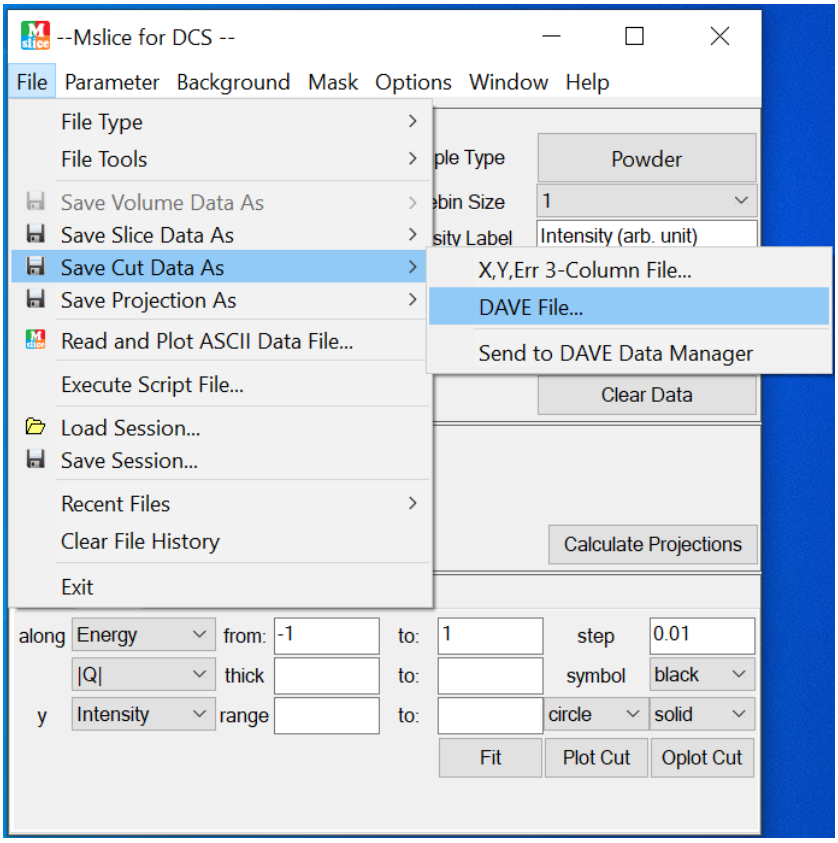


We can compare different data sets by loading new data and using “Oplot” to plot the data.

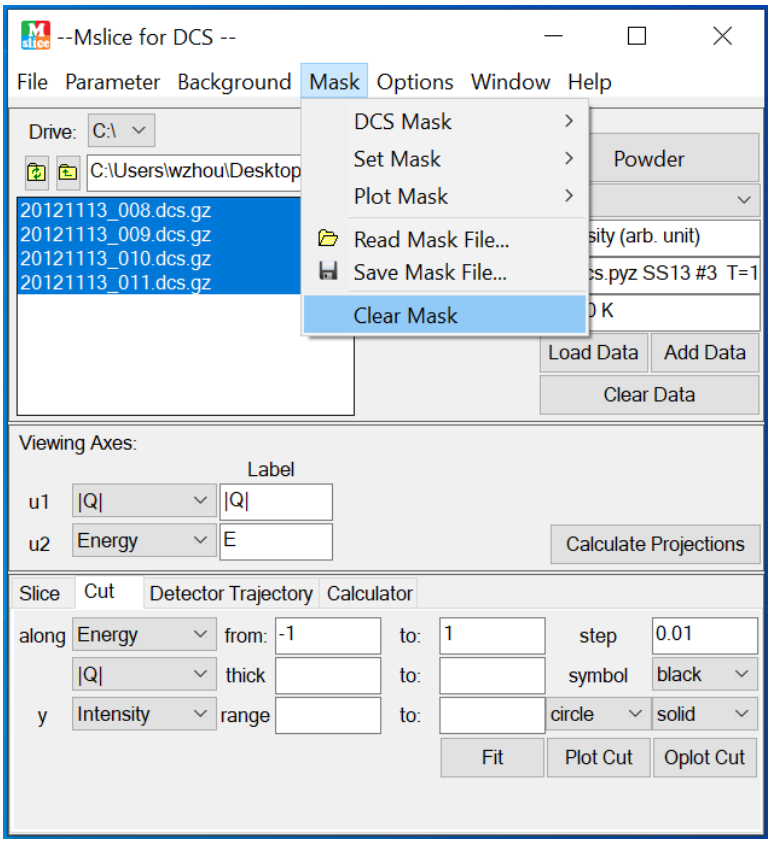




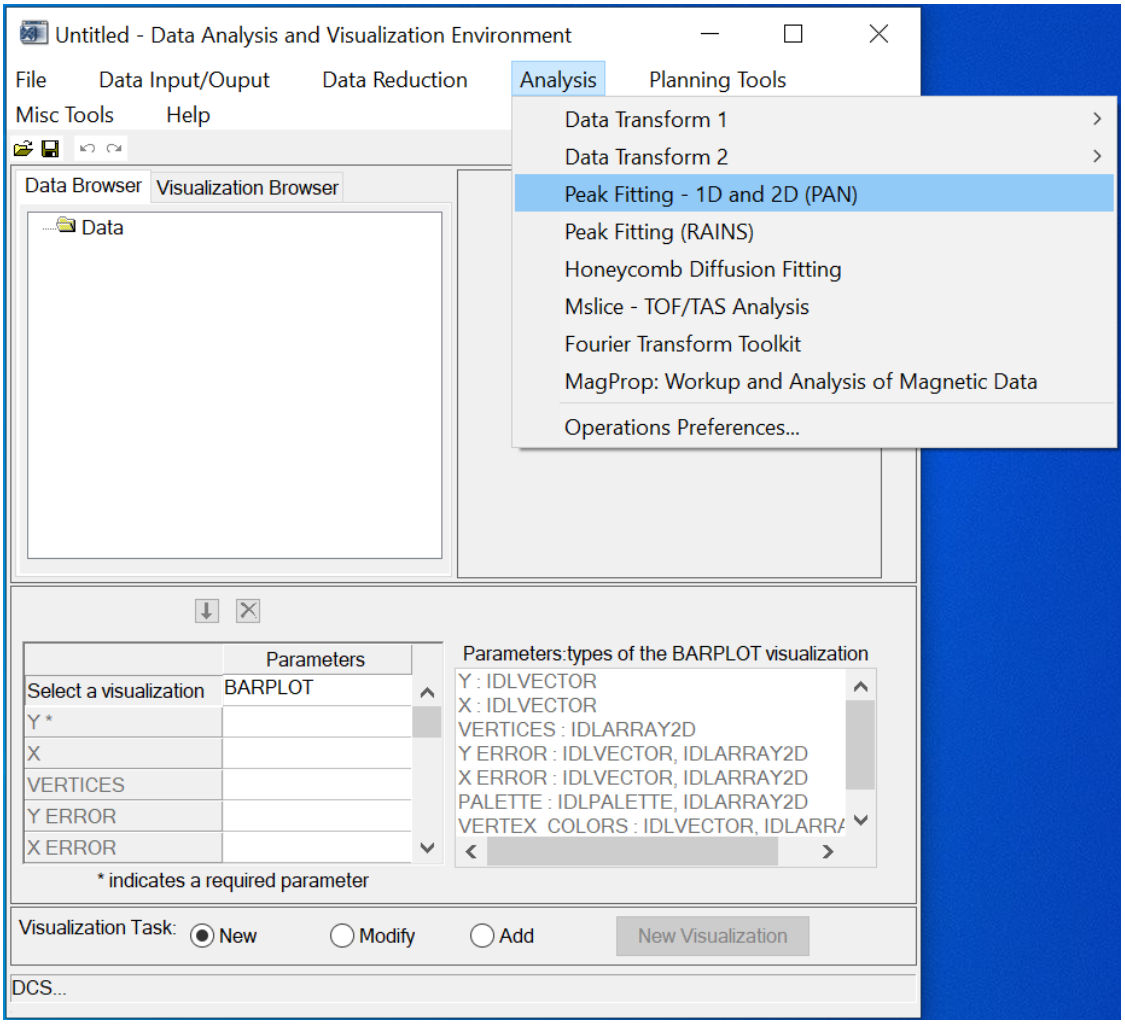
The “Cut data” can be saved as well.



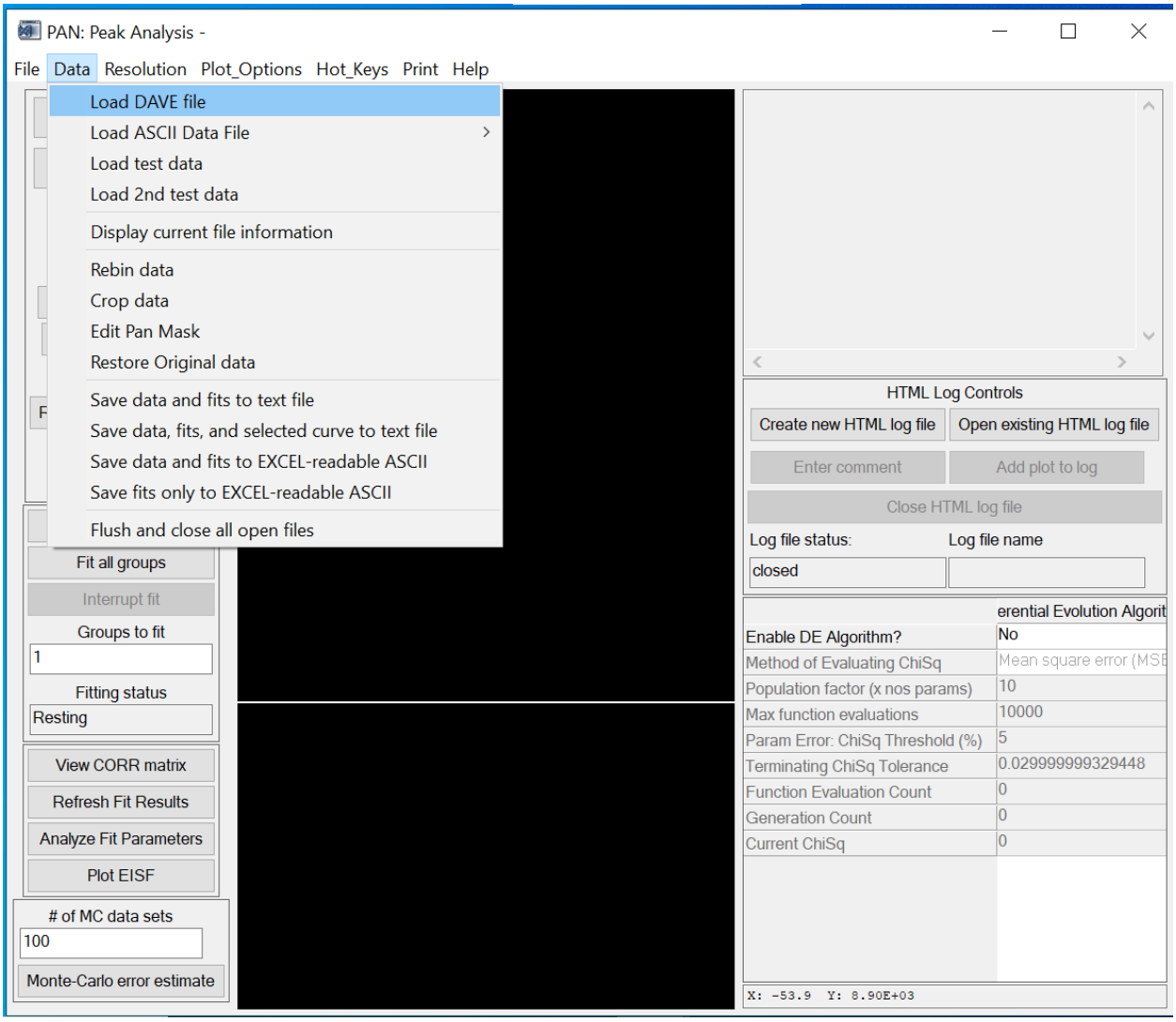
We also need to reduce the Vanadium data (to be used as instrument resolution). For Vanadium (no Bragg peaks), we don't want to use masks. Other than that, the procedure is the same.



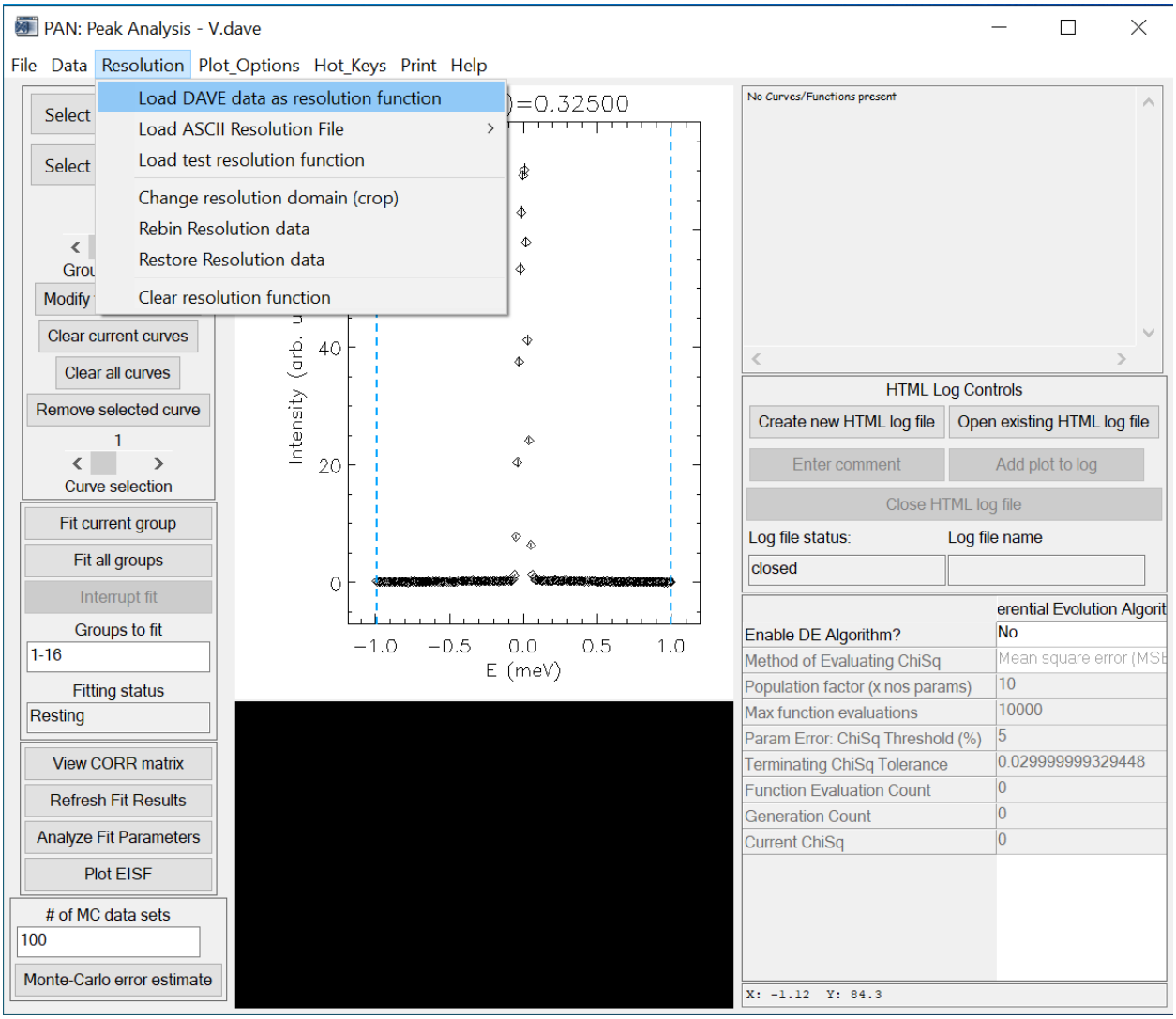
We use the PAN program for data analysis.



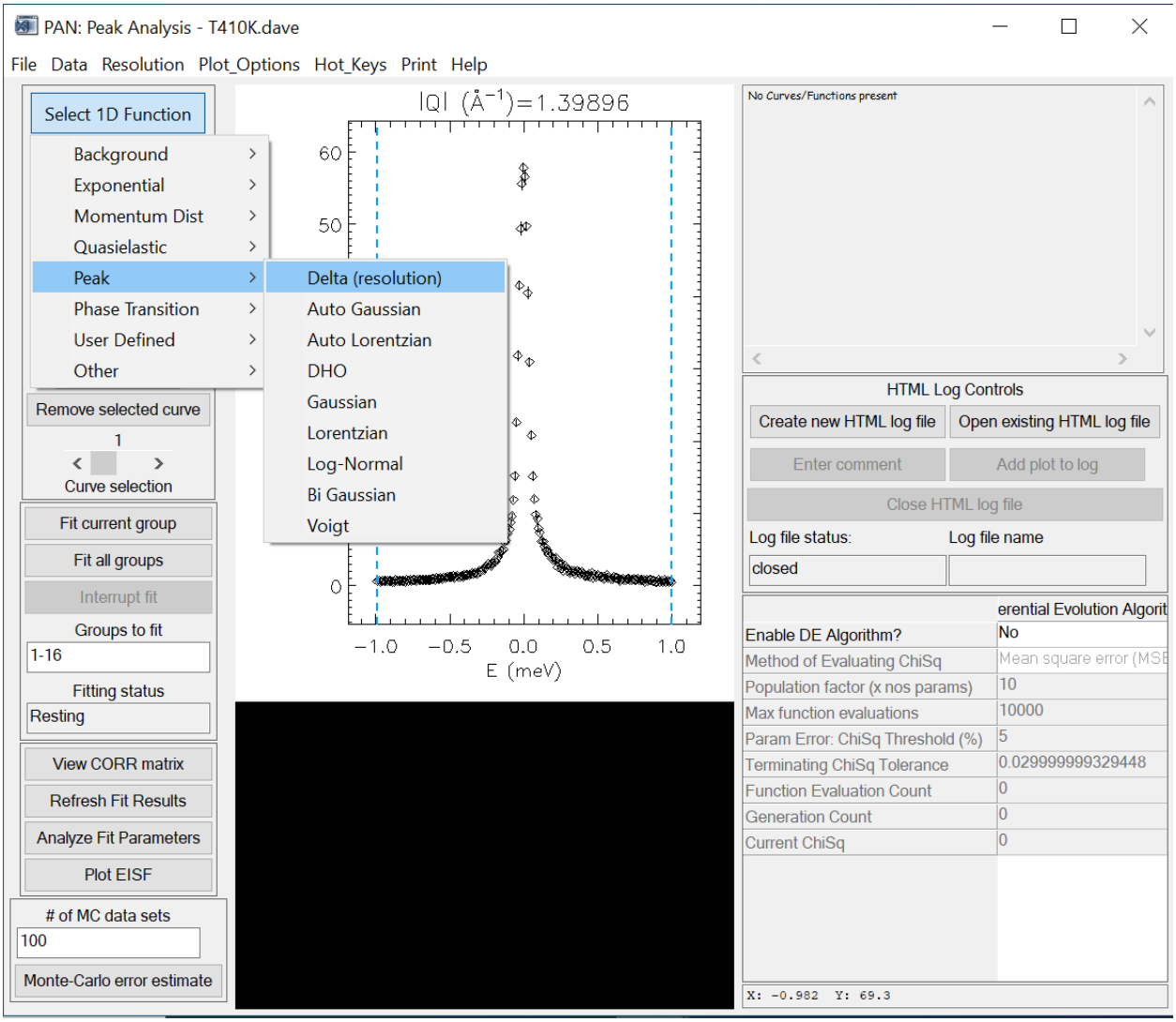
We first load the DAVE file of the sample.



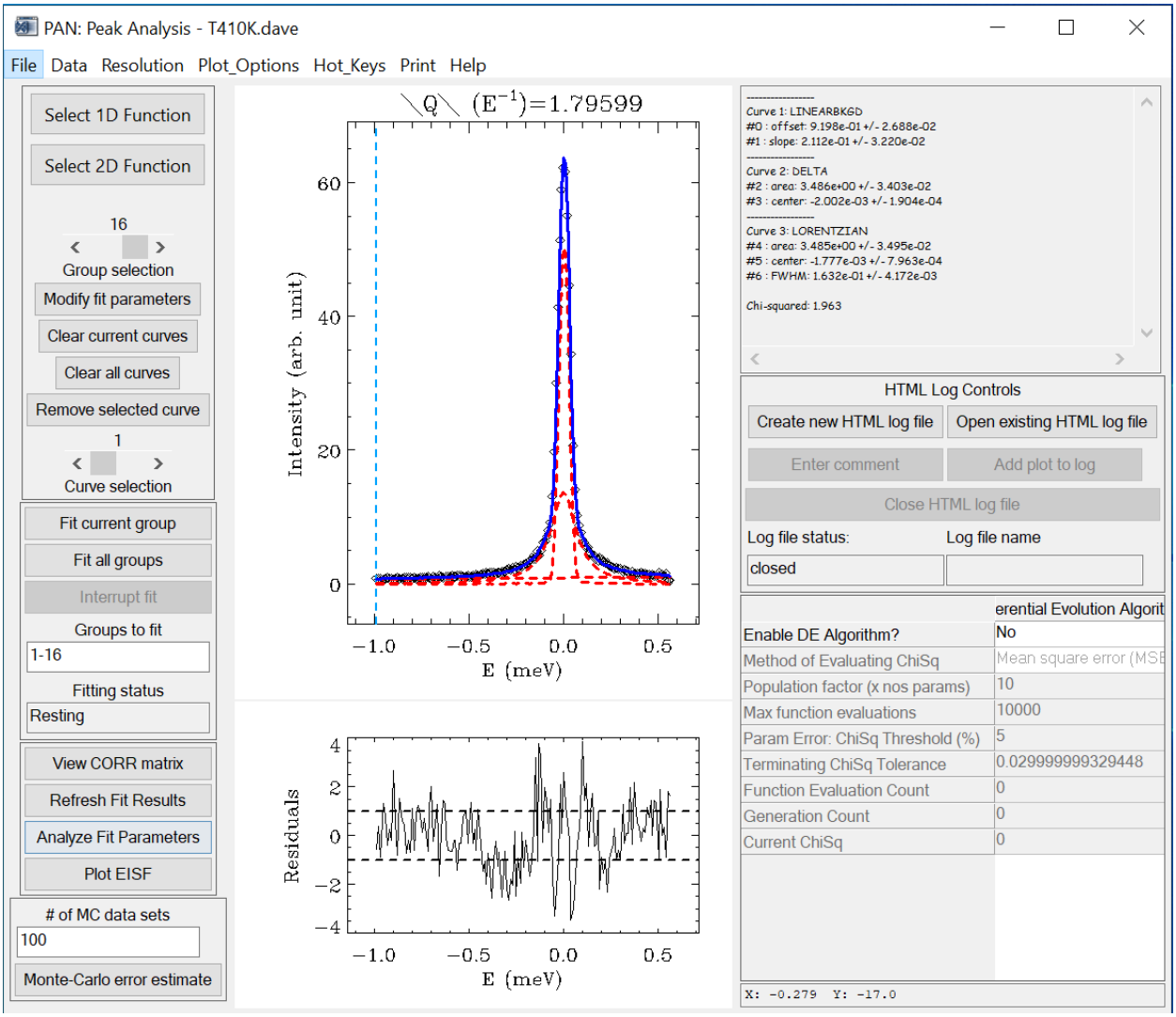
We then load the DAVE file of Vanadium (or the data file of the sample measured at very low T if it).

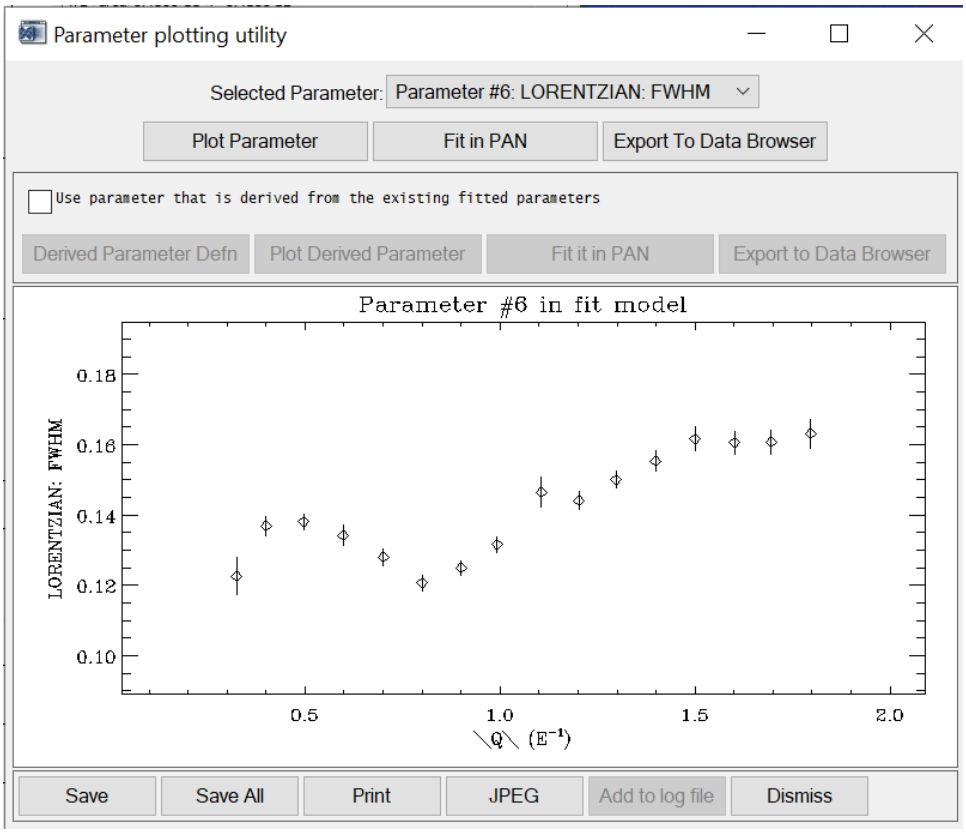


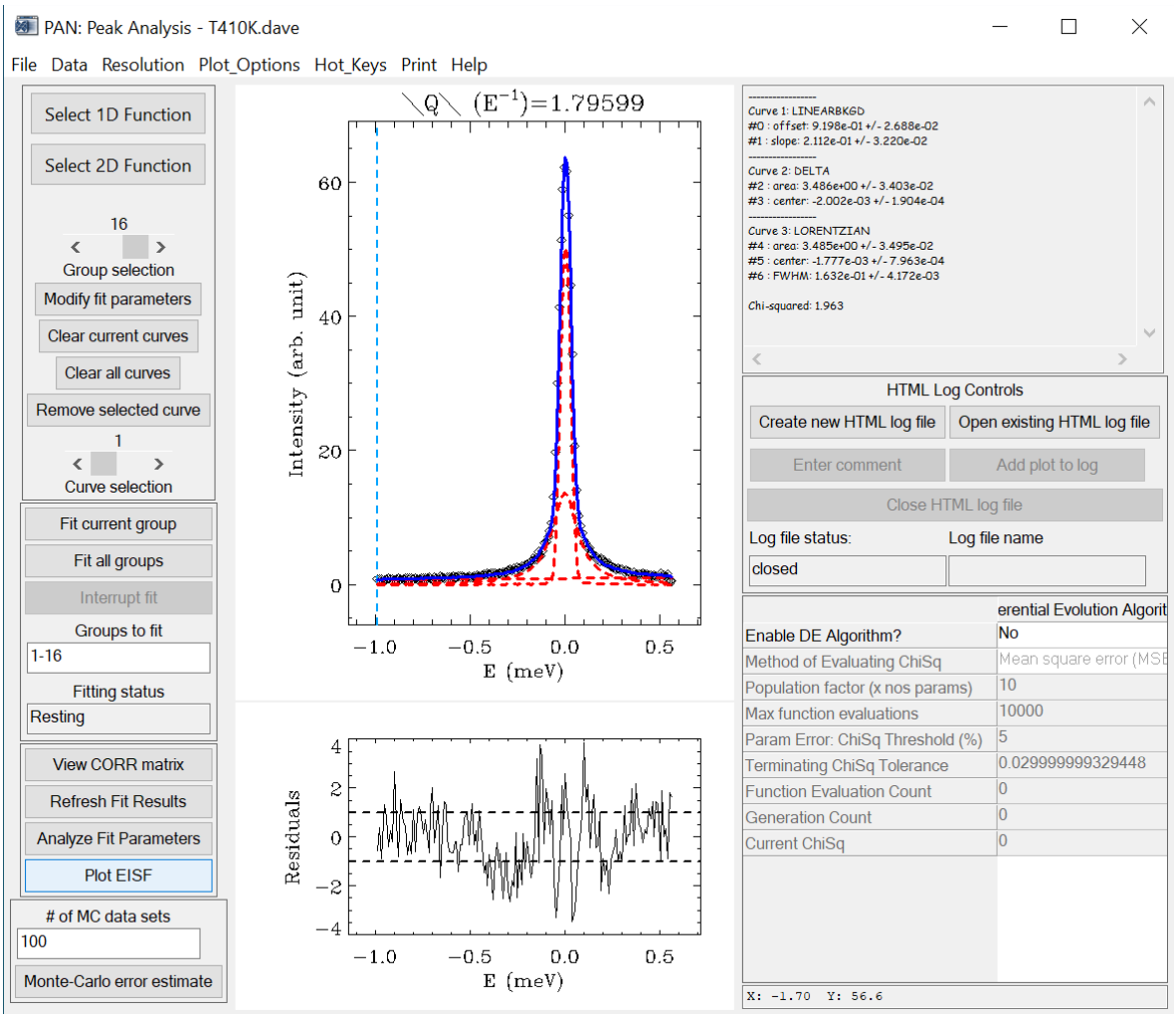
Now we can fit the data. In this case, we use a linear background, a Delta function and a Lorentzian function.

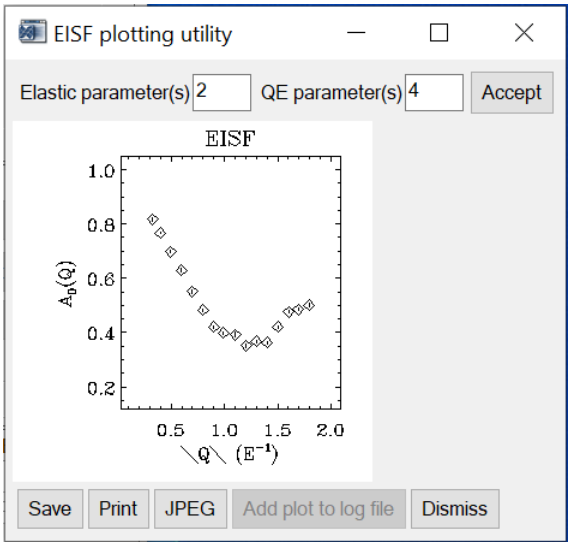


Once the data fitting is done, we can “Analyze Fit Parameters” and “Plot EISF”




Parameter plotting utility
Selected Parameter:
Parameter #6: LORENTZIAN: FWHM
Plot Parameter
Fit in PAN
Export To Data Browser
Use parameter that is derived from the existing fitted parameters
Derived Parameter Defn
Plot Derived Parameter
Fit it in PAN
Export to Data Browser
Parameter #6 in fit model
LORENTZIAN: FWHM
0.18
0.16
0.14
0.12
0.10
0.5
1.0
1.5
2.0
\Q\ (E⁻¹)
Save
Save All
Print
JPEG
Add to log file
Dismiss





We can further save the EISF data as an ASCII file, and fit the data to investigate its Q dependence etc.