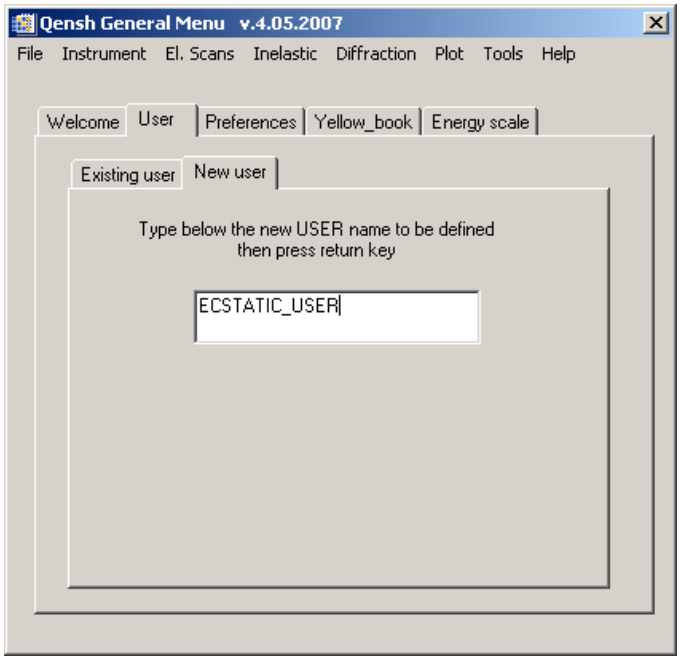
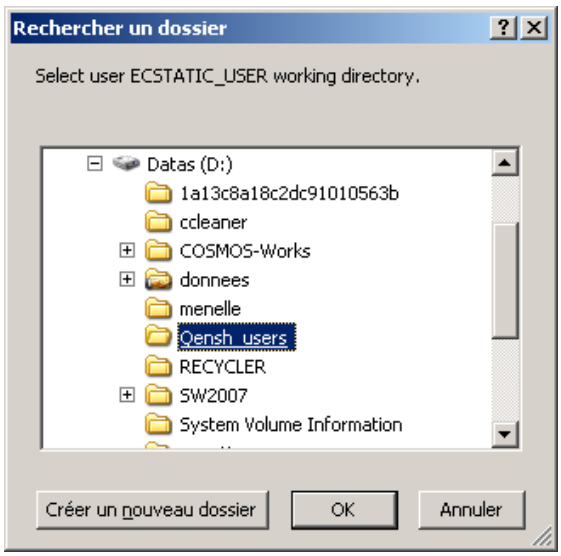
First steps for USING QENSH

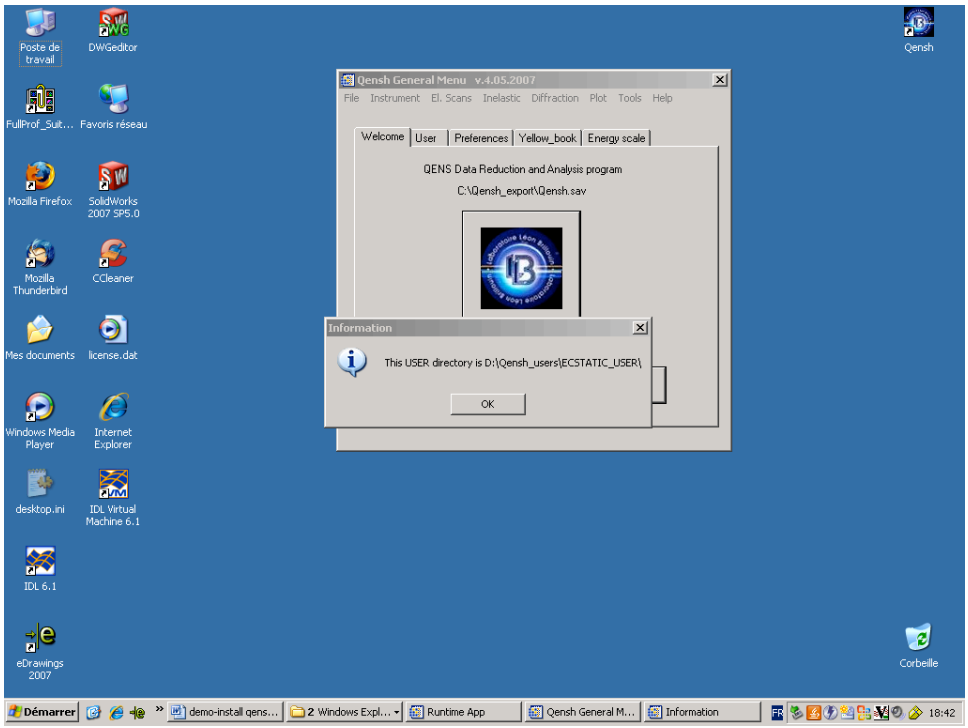
1) **Definition of a user** (in TAB User)



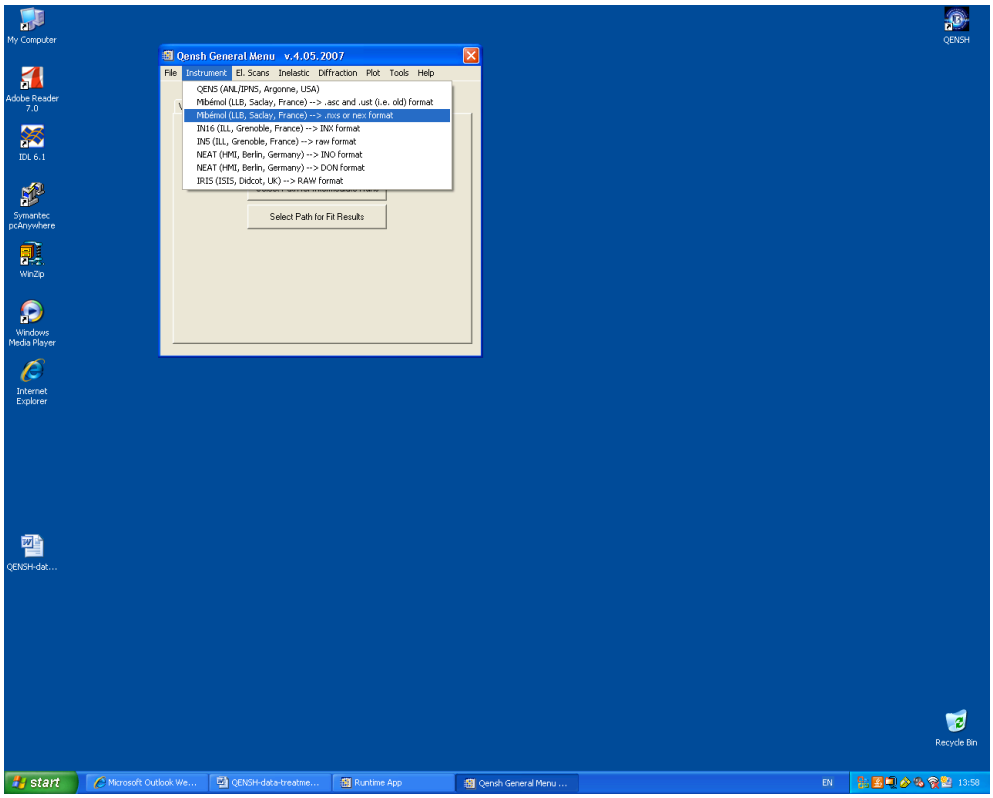
- Select 'New user' TAB and write down a new name (NOTE: no spaces in the name)
- Press Enter



- Select the D:\ drive, make a new directory 'Qensh_users', and select it
- Go back to the Welcome TAB, it will show now 'ECSTATIC_USER' at the bottom, if you click on 'ECSTATIC_USER', the following path to the user directory appears



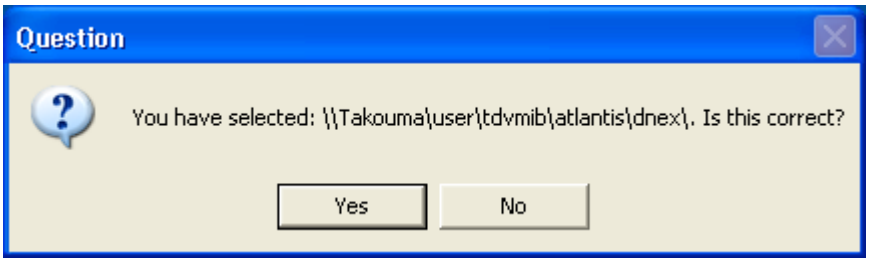
2) **Definition of instrument**



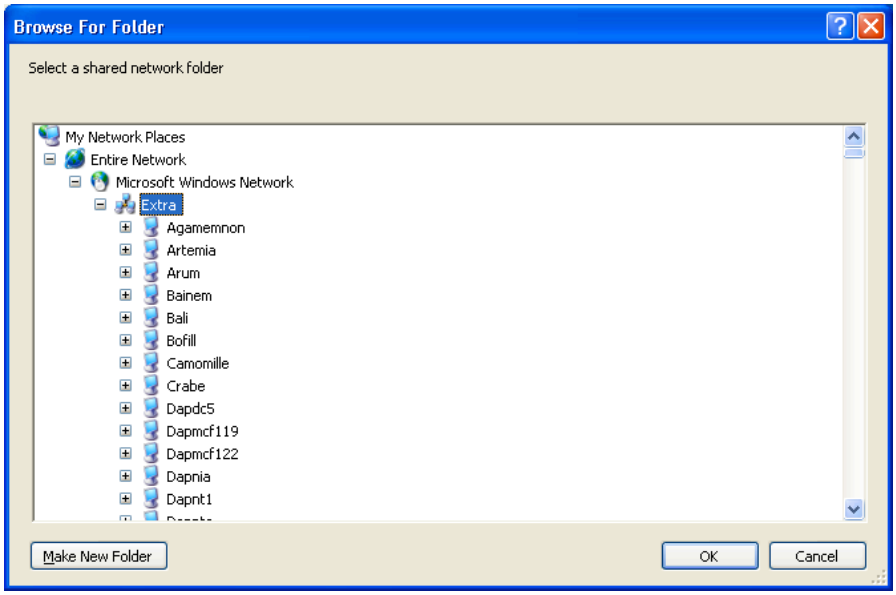
- Going to TAB Instrument – choose the appropriate instrument, all of the current data acquired on MIBEMOL are .nxs and .nex format

2) **Definition of pathways** (in TAB Preferences)

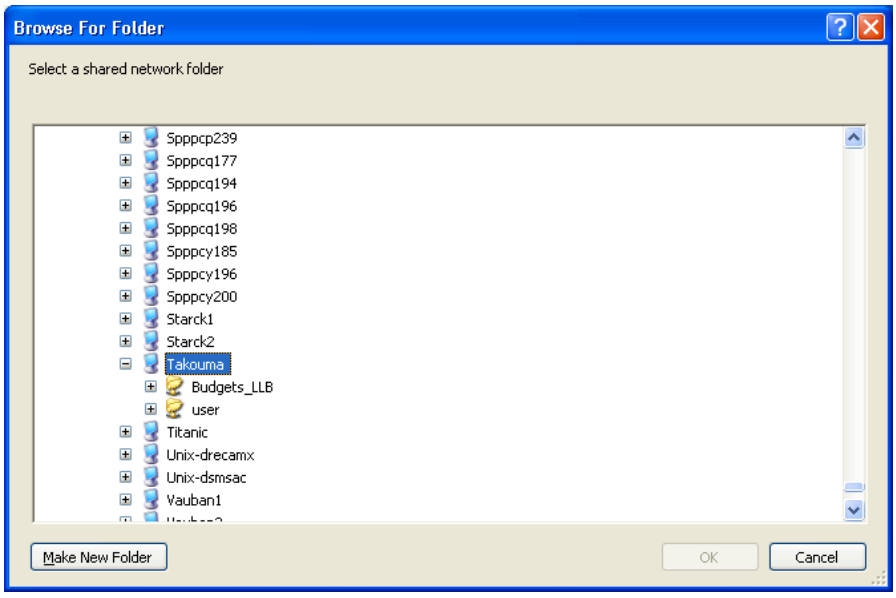
a) click on '**Select path for raw data'** and select a path



- When working in LLB, the raw data are stored in the above path. To get to takouma you need to select:



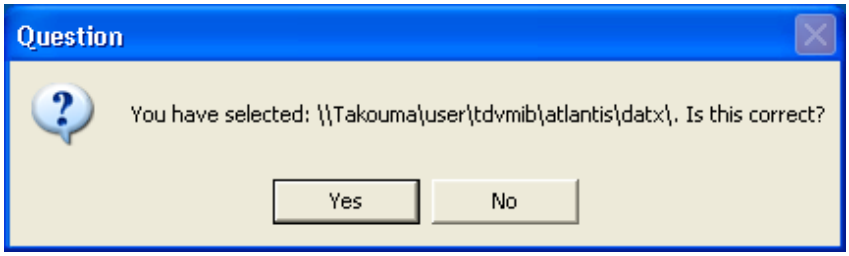
- Then scroll down to find ‘takouma’ and continue to select ‘user’ etc.



When working on PC other than in LLB you need to specify the path to where you saved the data locally. These are .nxs files.

b) click on **‘Select path for intermediate runs’**

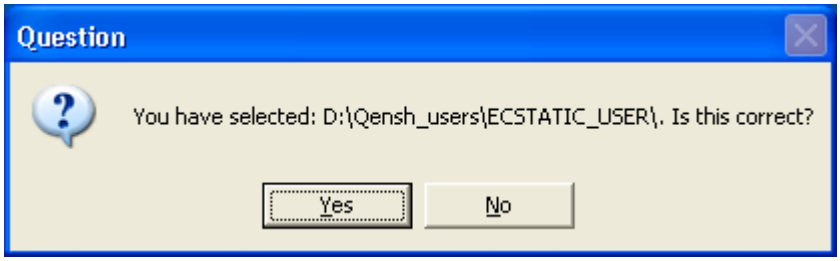
Again, when working in LLB the path to intermediate runs is:



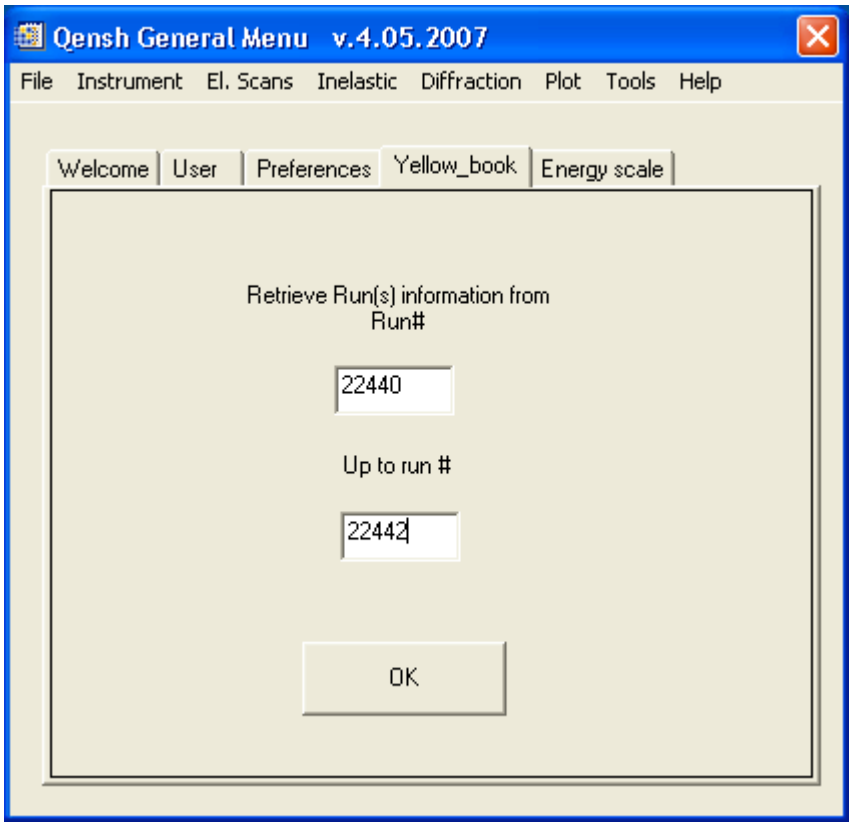
The intermediate files are called .nxs1, .nxs2 etc…

c) click on '**Select path for fit results**'

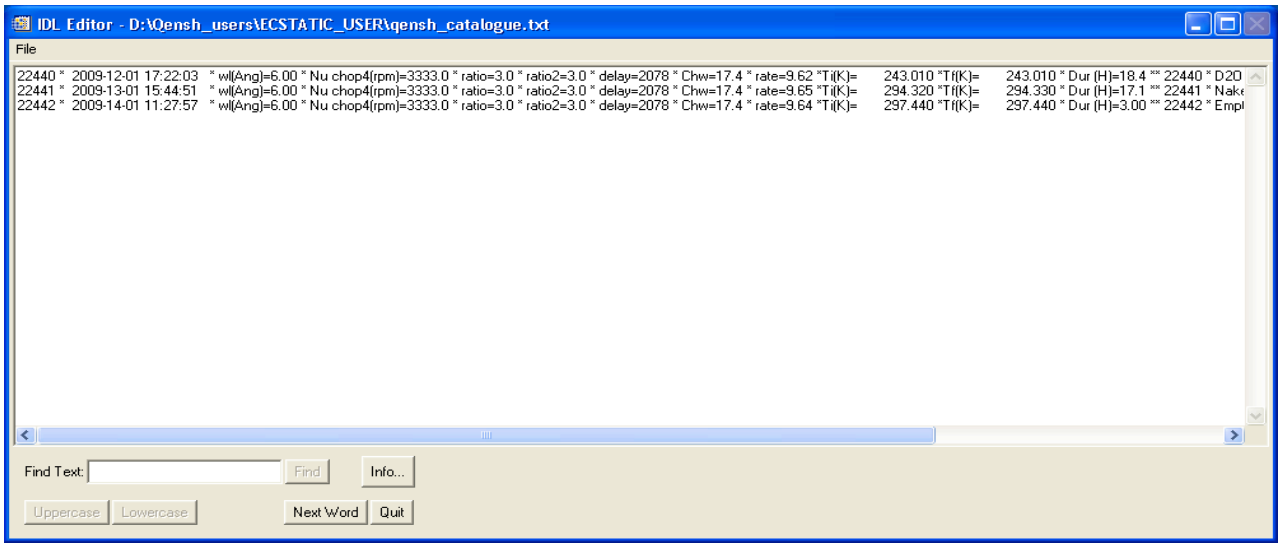
You should put the fit results in the user directory defined previously, i.e.:



3) **Looking up brief summary of run details**



- Go to the TAB 'Yellow_book' and enter the range of run numbers to be viewed, then click on OK, the following table with details shall appear. It contains the run number, date, wavelength, some chopper settings, temperature, duration and run title:

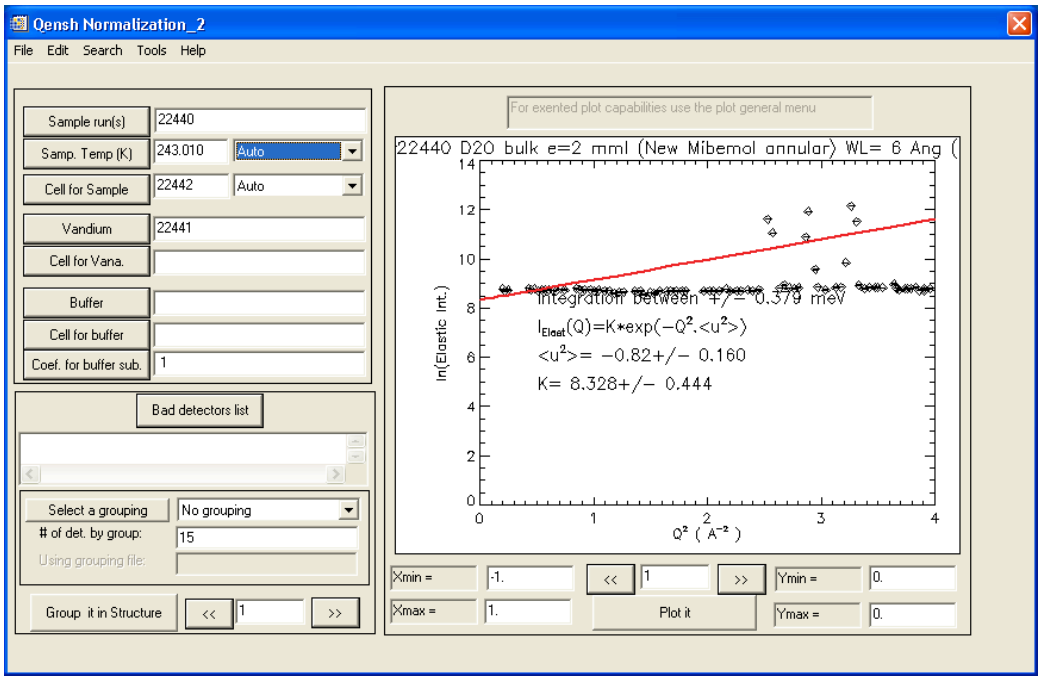


- Click on 'Quit' to close the table.

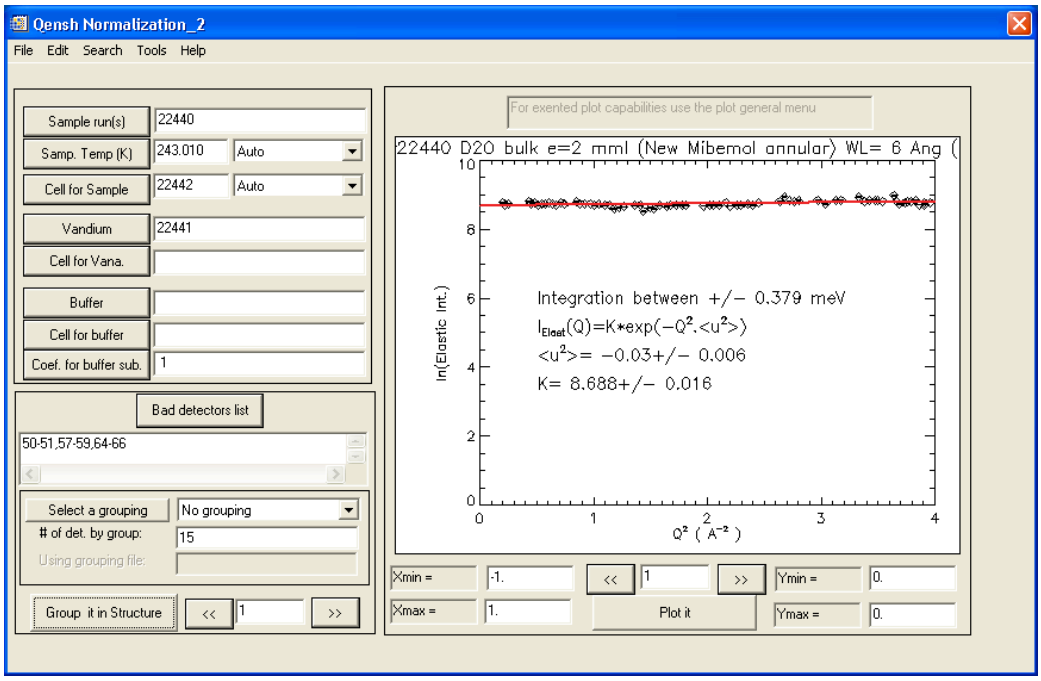
3) **Data Normalisation and Grouping** (in TAB Inelastic)

Need to group **sample** and **vanadium** at each wavelength
Sample: enter runs for sample, empty cell for sample, vanadium, empty cell for vanadium
Vanadium: enter vanadium and empty cell ONLY (in first two windows, in place of sample)

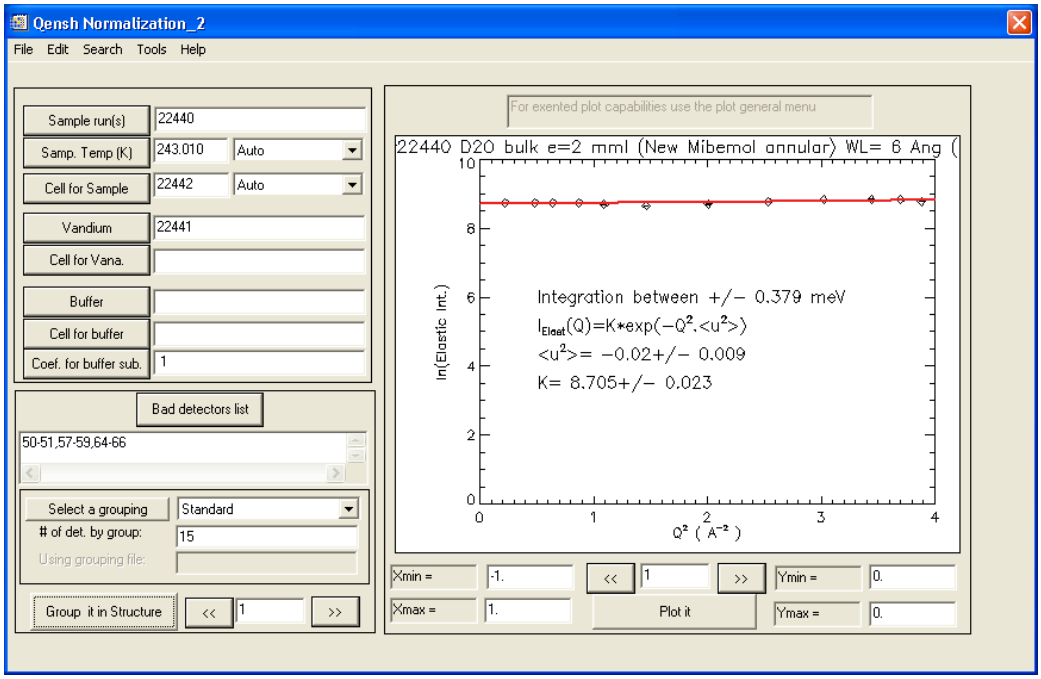
- Select no grouping (to view all 72 detectors), click Group in Structure (=Workspace) X, (there are 20 workspaces in total) – you shall see the following:



- If clear Bragg peaks appear, remove data by inserting numbers of Bad detectors (e.g. 10,11 etc) – in this example we had to remove 50-51,57-59,64-66, we see the end results as:



- Once you are satisfied that all bad detectors are removed, select Standard Grouping and rewrite the workspace X with grouped data (Click Group in Structure again), you shall see:

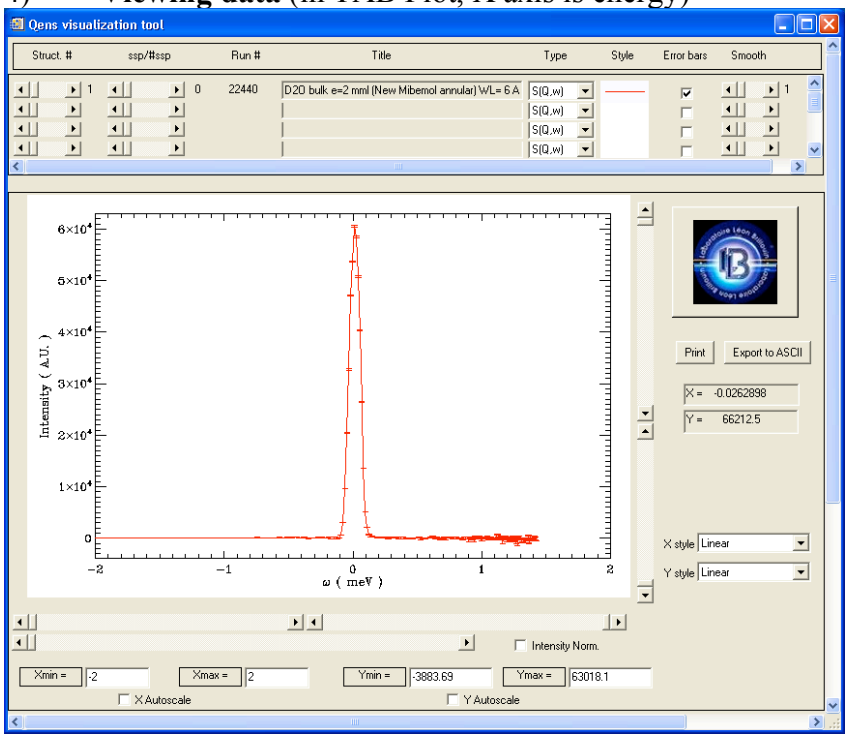


- In the above treatment for sample, vanadium is used to normalise the intensities of the sample signal. Grouped Vanadium signal by itself shall be used later in the fitting procedure to provide the elastic peak.
- Plot that appears on the RHS: Logarithm of the scattered intensity integrated between the limits shown as a function of Q^2. From a linear fit the following is obtained:

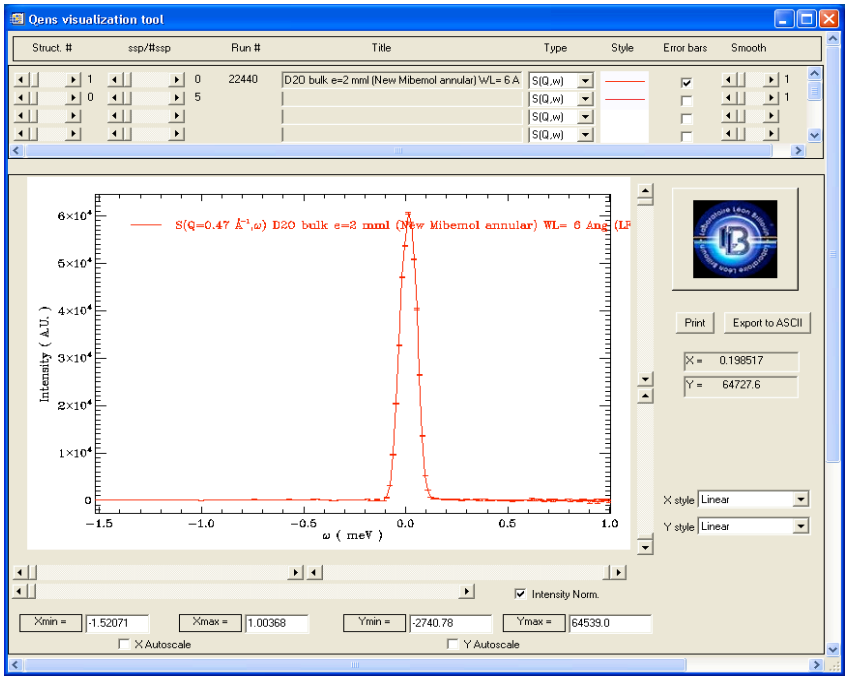
  $\langle u^2 \rangle$: slope (related to vibrational amplitude)

  K: y intercept, i.e. logarithm of the total scattered intensity at Q=0, together with the mass of the sample it is used for subtracting signals of reference samples, e.g. dry and wet samples.
- Close the 'Qensh_normalization_2' window by clicking on the cross top RHS.

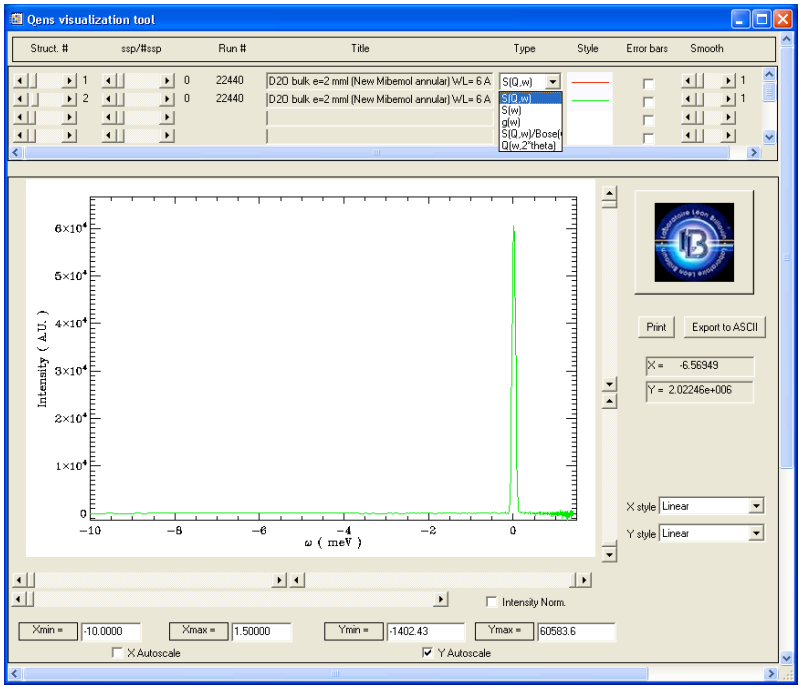
4) **Viewing data** (in TAB Plot, X axis is energy)



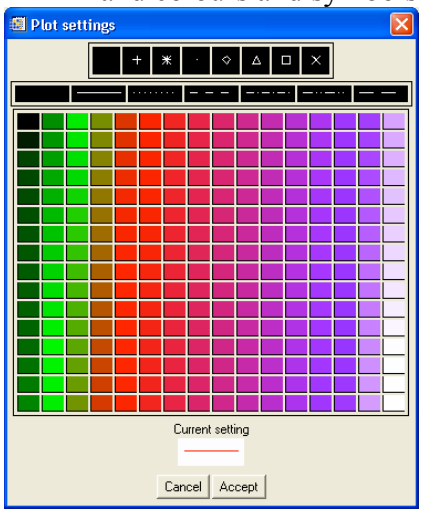
- Scroll on the 'Struct' to find the workspace desired (maximum 20 workspaces)
- Selecting the 'Error Bars' option allows the visualisation of error bars for individual experimental data points.
- Selecting 'Intensity Normalisation' below the graph window: all the graphs in the window shall be normalised to the same value at the maximum.
- Each Structure contains several subspaces ('ssp'). Each 'ssp' corresponds to a S(Q,w) curve at a different Q. To visualise which Q each 'ssp' corresponds to doucle-click on the graph, a legend will appear mentioning the Q. To get rid of the legend, hold Alt and double click.



- You can also visualise the S(w), i.e. S(Q,w) integrated over all Qs, see in the options 'Type':



- Double clicking on the 'Style' for a given Workspace, brings up the following menu and colours and symbols can be changed:

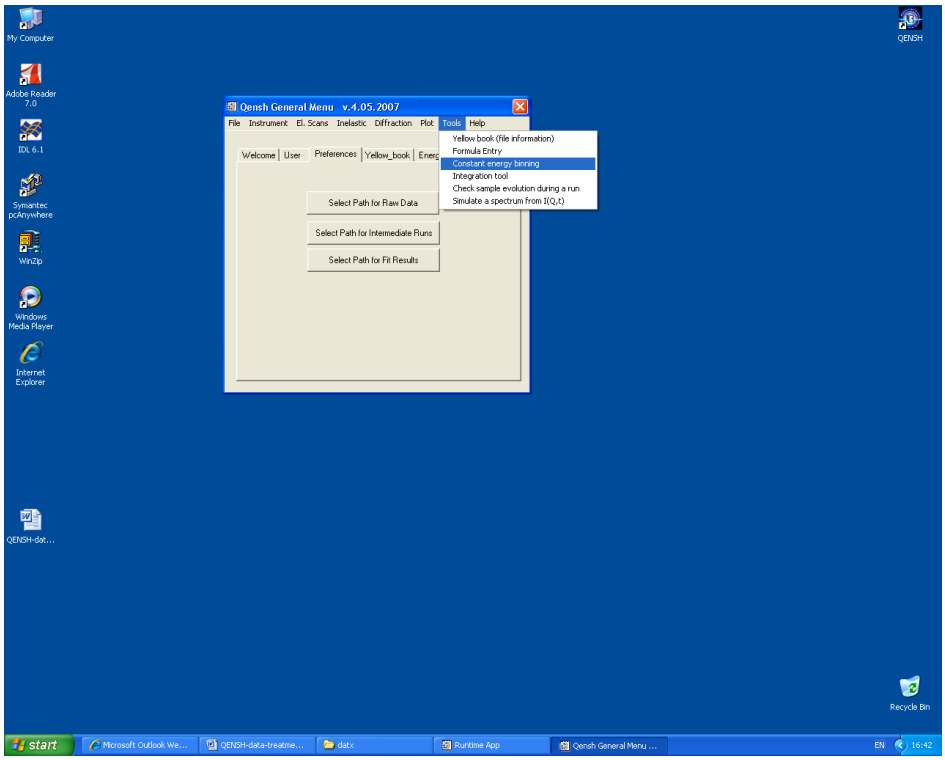


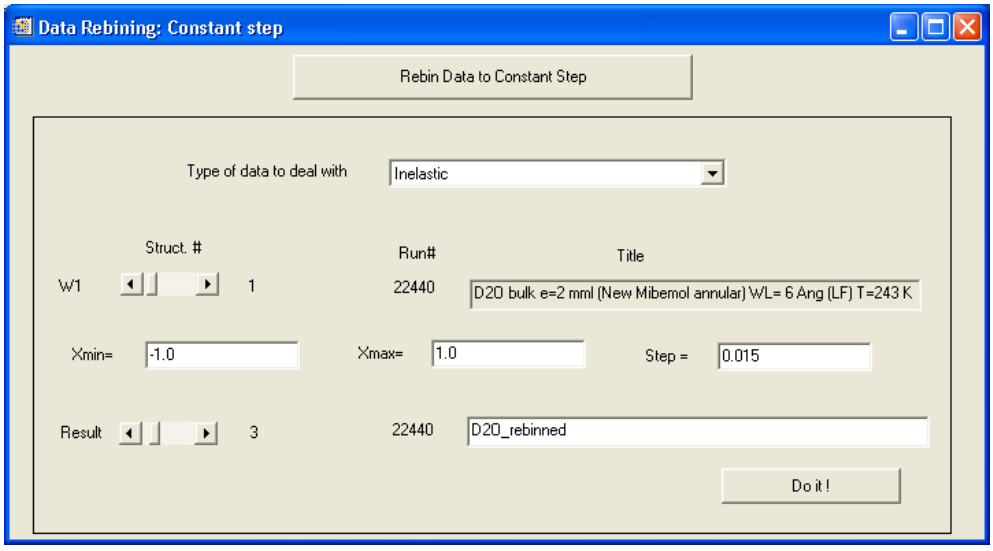
After general inspection of data, zoom in and determine spacing between successive points. Determine a suitable zone for analysis around elastic peak (maximum 1800 times the spacing found). – all this information is necessary for the next step of constant energy binning.

5) **Constant energy binning** (in TAB Tools)

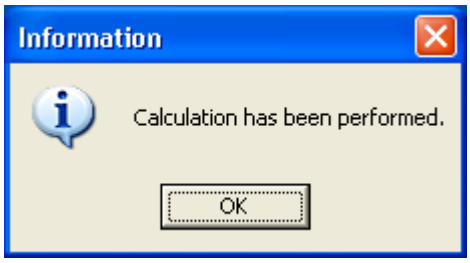
Why do we do this? The S(Q,w) data is collected at irregular energy intervals (it is collected at regular time intervals which, when transformed to energy, results in irregular energy

intervals). We need to 'rebin' each S(Q,w) to a constant energy spacing. This will allow a FFT of the data set, which is necessary if any data fitting is to be carried out.

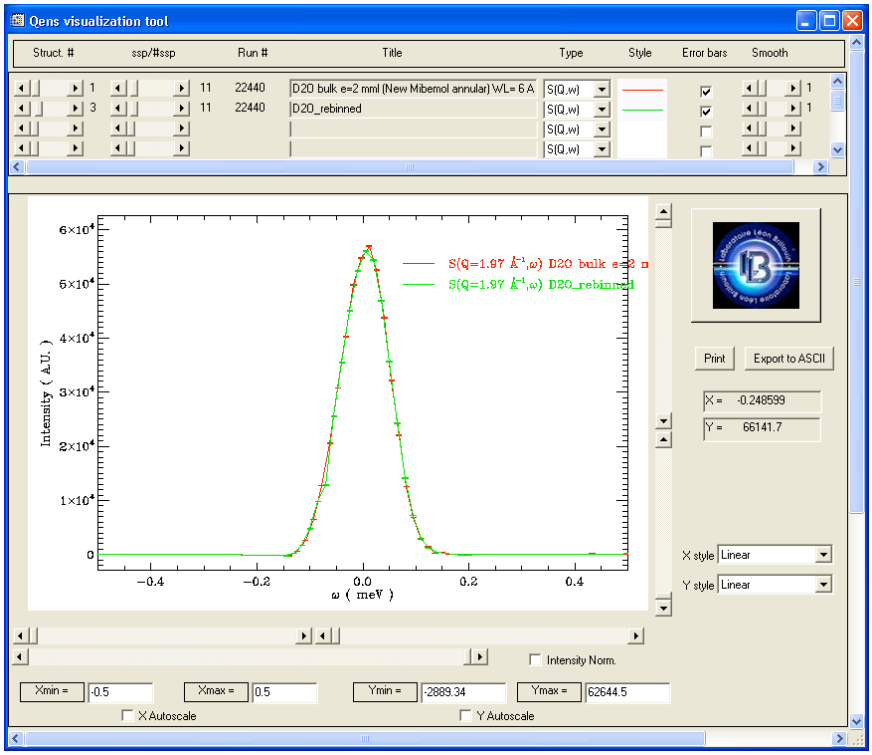




- Select type: Inelastic
- Enter the max, min, step determined previously (this is in units of meV) NOTE that the maximum number of points possible is 1800. An error message appears if you go over that number.
- Choose a new workspace for binned data and insert a name for the rebinned data in the window provided. When carried out the following message appears.



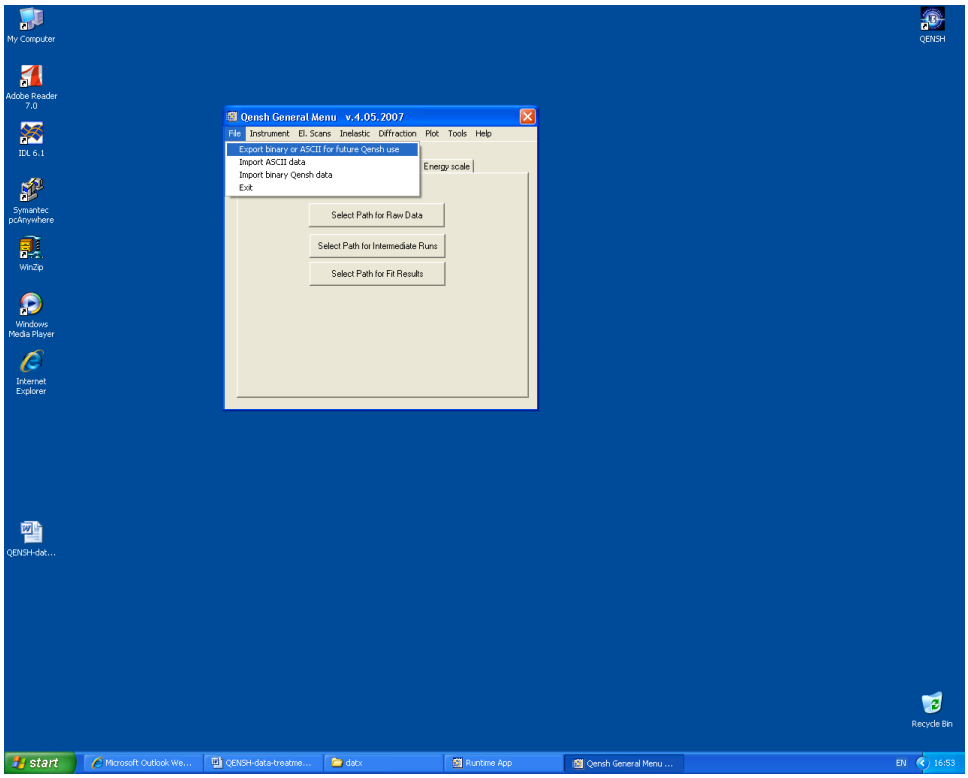
Need to do binning for both SAMPLE and VANADIUM. At the end of rebinning you need to check that the procedure has not distorted the data. So visualise both the original and rebinned data together:

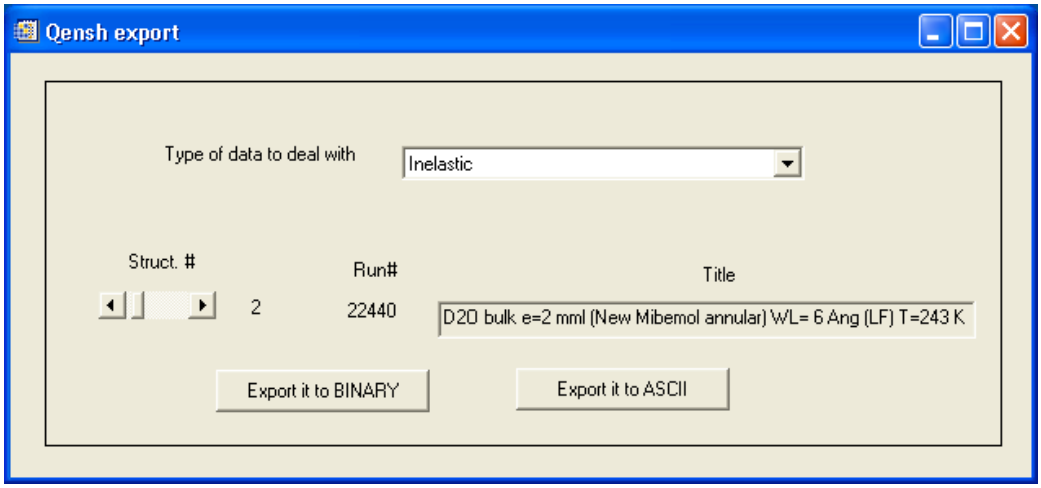


- The above shows a reasonable constant energy binning, the green and red curves are almost identical.

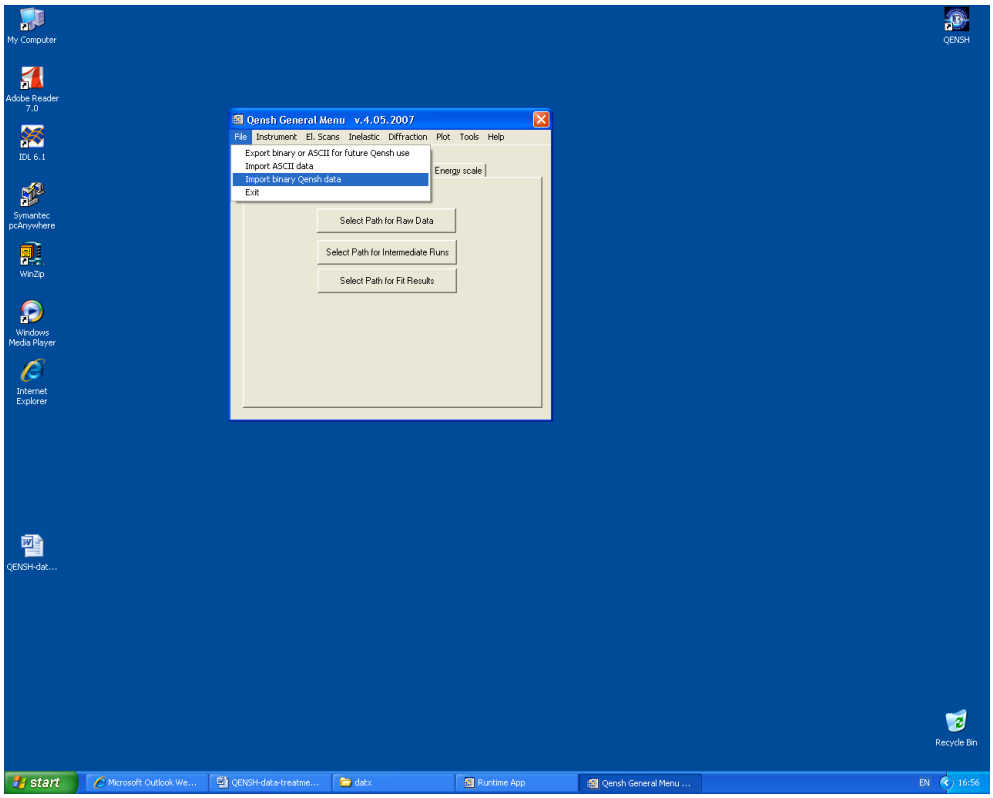
6) **Exporting binned data for future fitting** (TAB File; Export ../Import..)

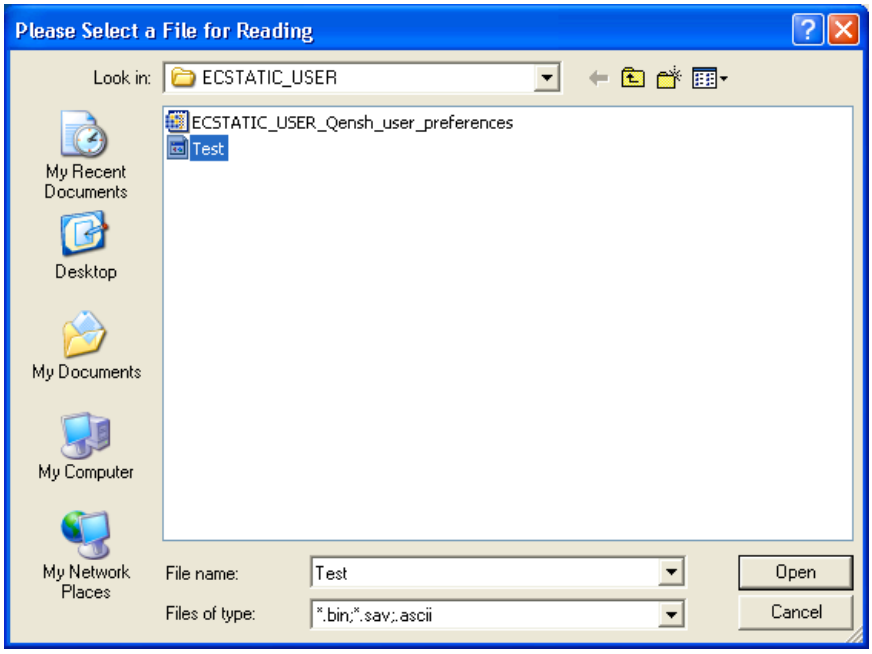
In order not to have to repeat the procedures of data normalisation and constant energy binning every times Qensh is launched, the normalised and energy binned data (both sample and vanadium) can be exported into a binary file, that can later be imported and fitting carried out directly afterwards.



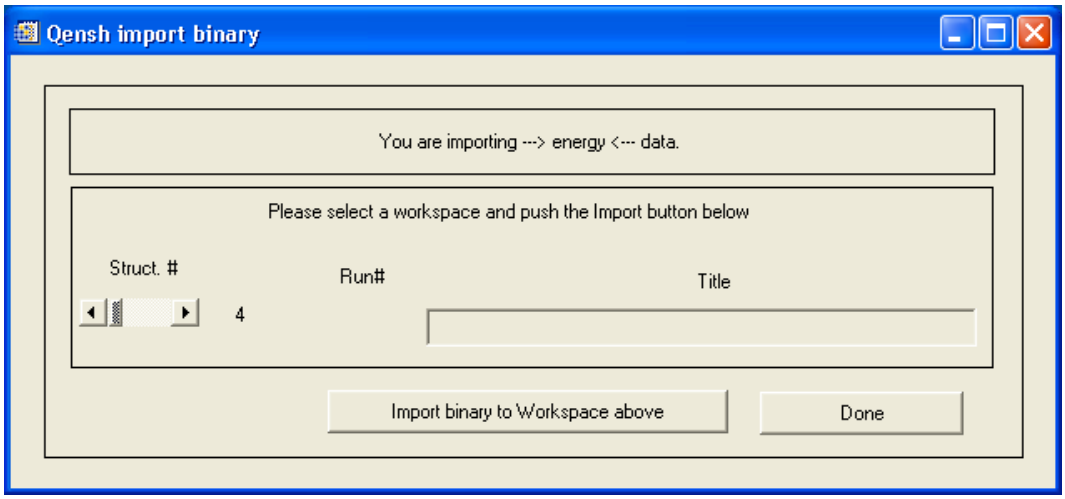


- Type: Inelastic
- Scroll to the workspace desired (NOTE the name CANNOT be changed at this stage) and click on ‘Export to BINARY’
- To Import data at a next session of Qensh:



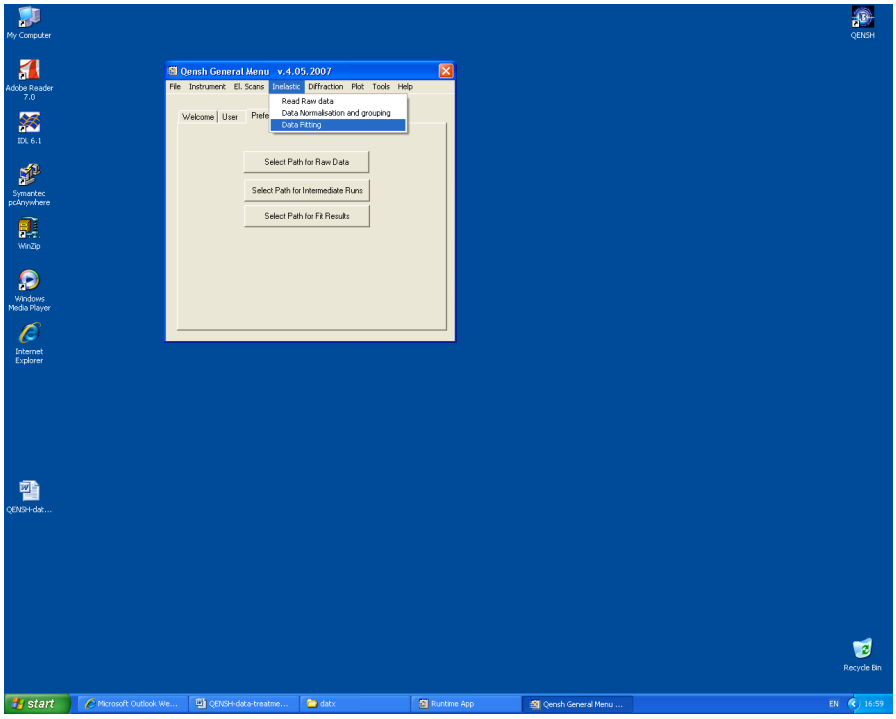


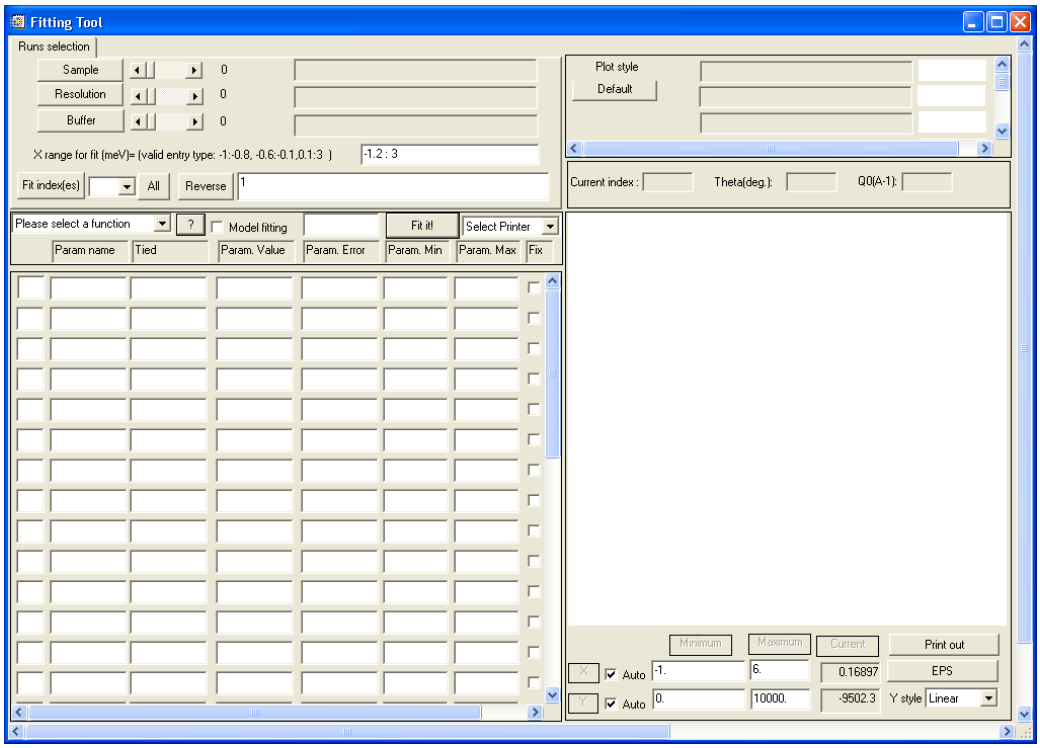
- Choose the binary file exported previously and click on Open



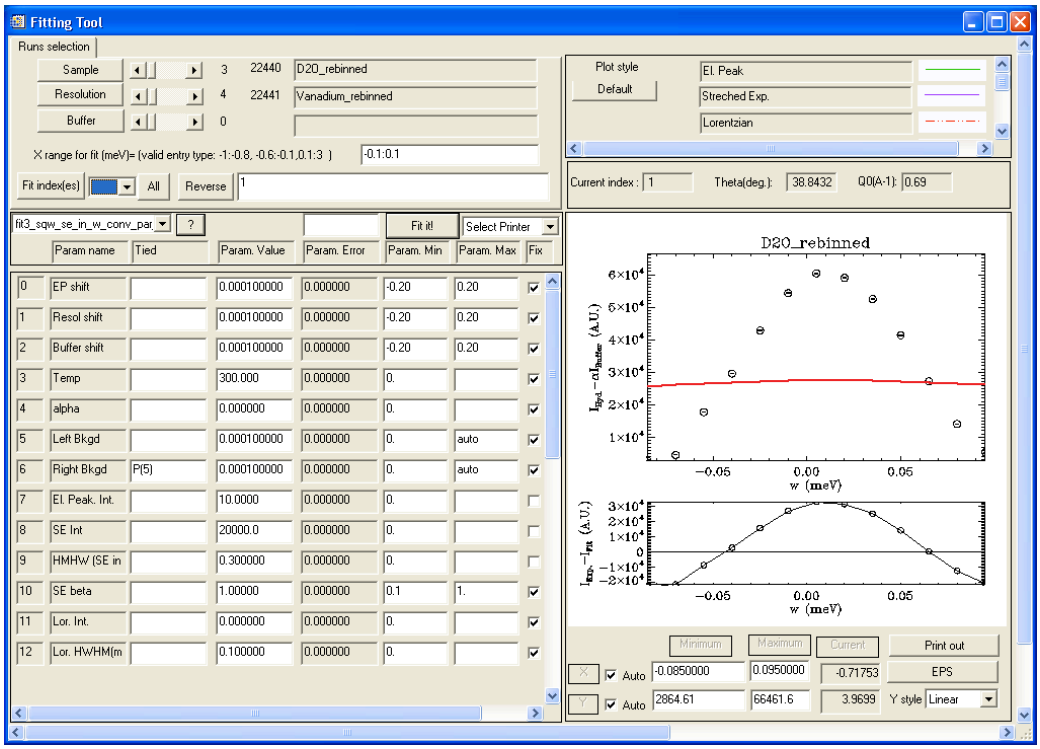
- Scroll to an empty Workspace and click on ‘Import binary’

7) **Data fitting** (TAB Inelastic; Data fitting)





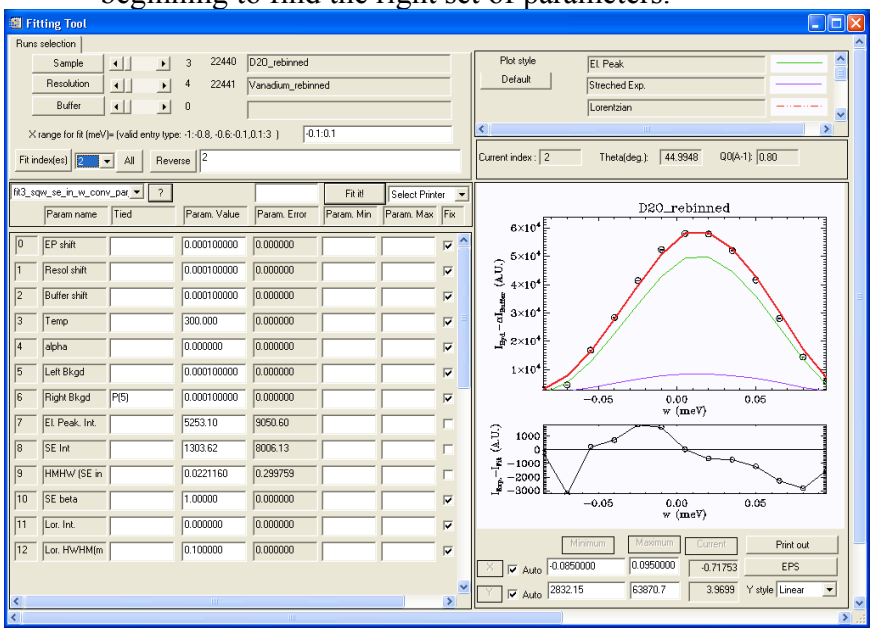
- Enter **normalized and rebinned data** for sample and vanadium (possibly buffer)
- Define x-range for fit, this has to be at most the range over which the data has been rebinned
- Select fitting function – the following shall appear:



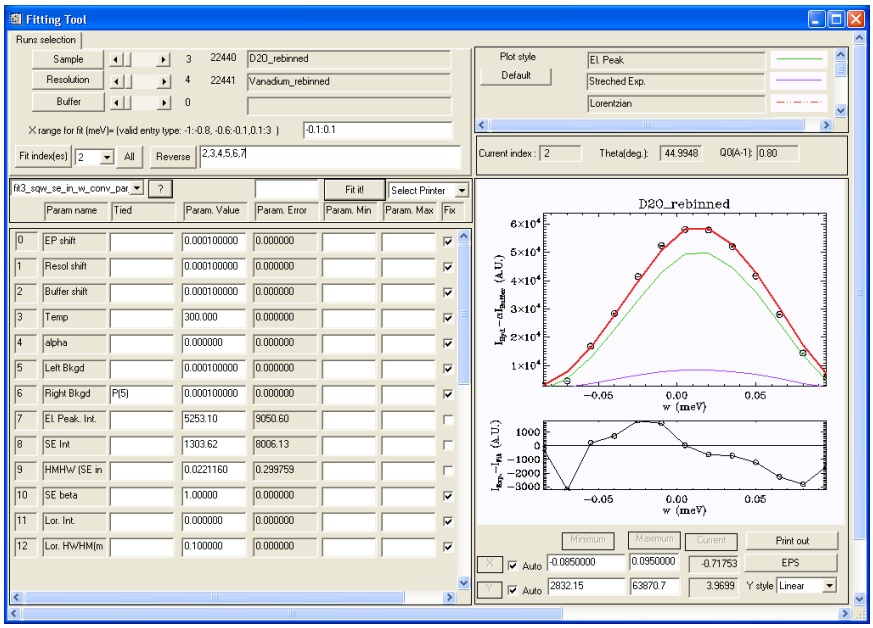
- Now choose a fit index out the scroll down menu to fit a single S(Q,w). The Q that you are fitting appears above the graph on the RHS.
- Modify the initial values for the fitting parameters. Press enter after each modification so that the new value is taken into account, the graph on the RHS changees

accordingly, telling you what the modelled signal looks like with the parameter entered.

- Then press 'Fit it!' – after some iterations, the following appears, with the modelled signal (in red) close to the measured signal (in black). If the two signals are nowhere near, need to start with a different set of initial parameters – need to play with it at the beginning to find the right set of parameters.

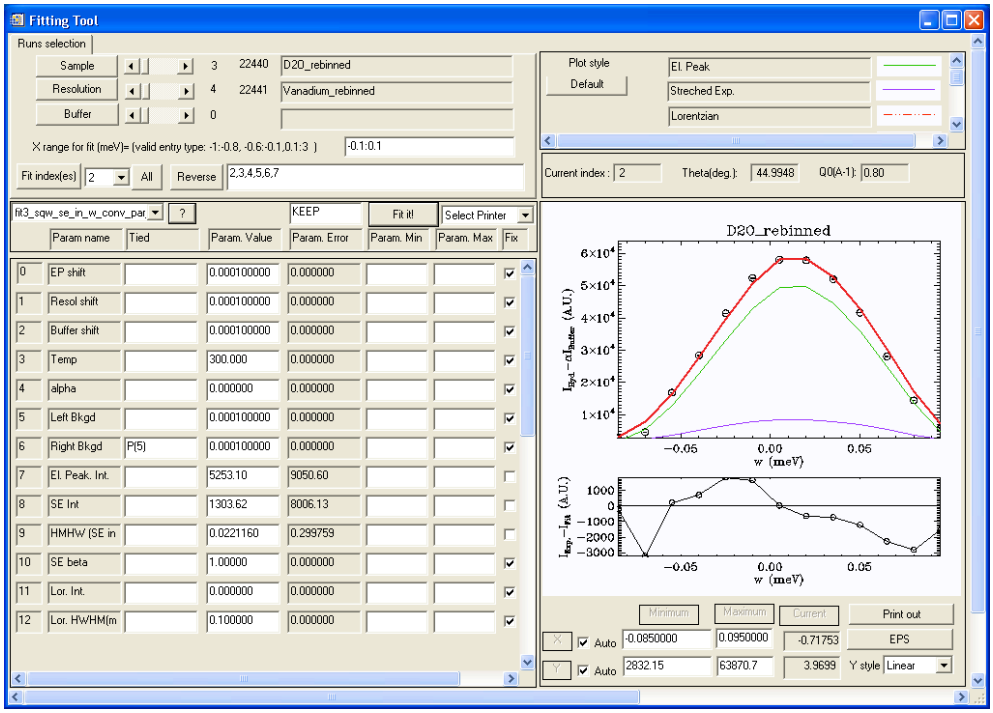


- If you wish fix certain parameters throughout the fitting, just put in the desired value (followed by enter) and then check the box at the end 'Fix'.
- You can tie parameters to the same value, such as is done above for the Right and Left Background, i.e. parameter 6 is tied to parameter 5, P(5).
- You can insert min and max values for any parameter (followed by enter).
- You can also fit several S(Q,w) curves in a row, by specifying the sequence in the box to the right of 'Reverse' (clicking on the 'Reverse' button reverses the sequence that you entered):



- Every time you press 'Fit it!' a results file is formed in your user directory with the resulting values of the fit (in ASCII format) and a figure (a .ps file). Most of these files

you shall not need, as several tries are usually necessary to arrive at a good fit. To note which files to keep you can enter a note in the window to the LHS of ‘Fit it!’, this note shall be appended to the name of the file:



THE END