First steps for USING QENSH (version 21 Jul 2009)

NOTE: The most recent version of QENSH can be downloaded from the MIBEMOL webpage: http://www-llb.cea.fr/en/Phocea/Page/index.php?id=21

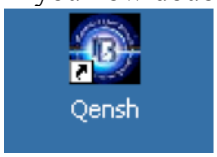
Overview of QENSH:

QENSH is a data treatment program for time-of-flight (TOF) quasi-elastic neutron scattering data. Raw TOF data comes in the form of scattered intensity as a function of scattering angle and time, i.e. $S(2\theta,t_{TOF})$. QENSH can read the raw data of several TOF spectrometers (from LLB, ILL, HMI, IPNS, ISIS). The general principle of QENSH is to read in a set of raw data into one of 20 workspaces and carry out later on various operations (plotting as function of energy, Q, angle…, energy fitting etc.) on these workspaces.

The following document is presented in several parts:

- **Definition of a user**
- **Definition of instrument**
- **Definition of pathways** (for raw data)
- **Looking up brief summary of run details**
- **Read raw data, in time-of-flight**
  - visualising raw data prior to any conversion and treatment
- **Elastic Scans**
  - initial treatment of samples to identify the temperature corresponding to an onset of some type of motion
- **Data Normalisation and Grouping**
  - preparation of data for the analysis of detailed quasi-elastic broadening, conversion into $S(Q,\omega)$.
- **Viewing data**
  - viewing normalised and grouped data
- **Constant energy binning**
  - necessary step prior to fitting of quasi-elastic data
- **Exporting binned data for future fitting**
  - saving normalised, grouped and energy binned data, ready to be fitted
- **Formula Entry**
  - some simple operations possible to carry out on data sets, if needed
- **Data fitting**
  - detailed fitting of quasi-elastic broadening

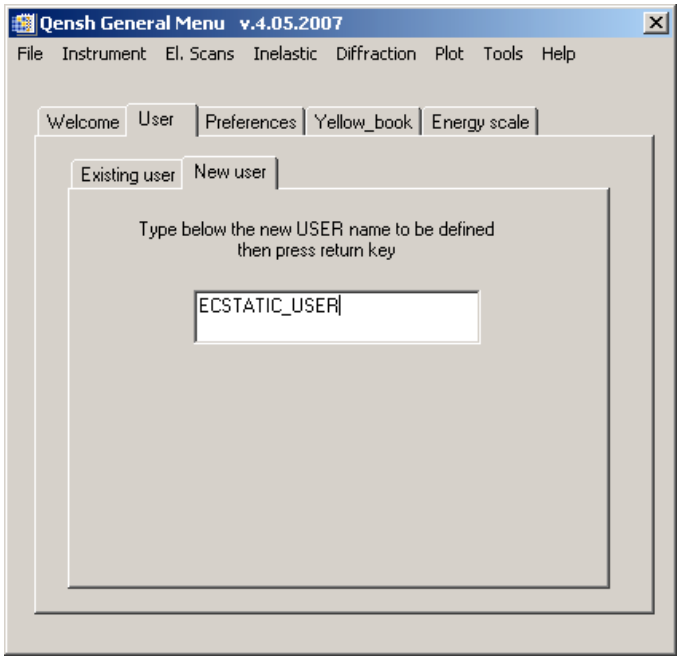
If you now double click on



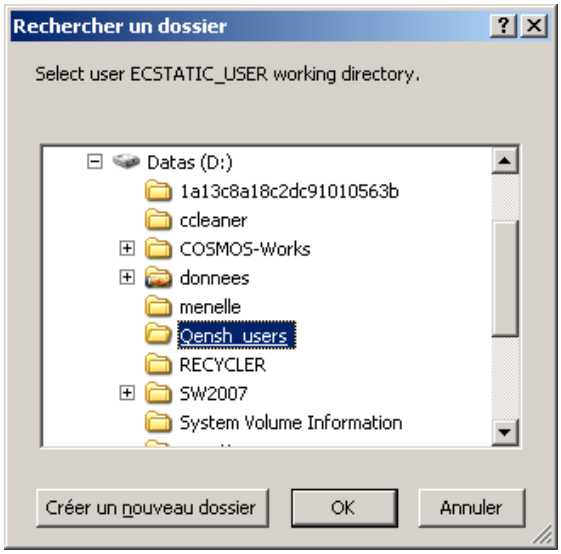
the following appears

- It can be that the above message appears, it is OK, read it and follow the instructions it gives you!

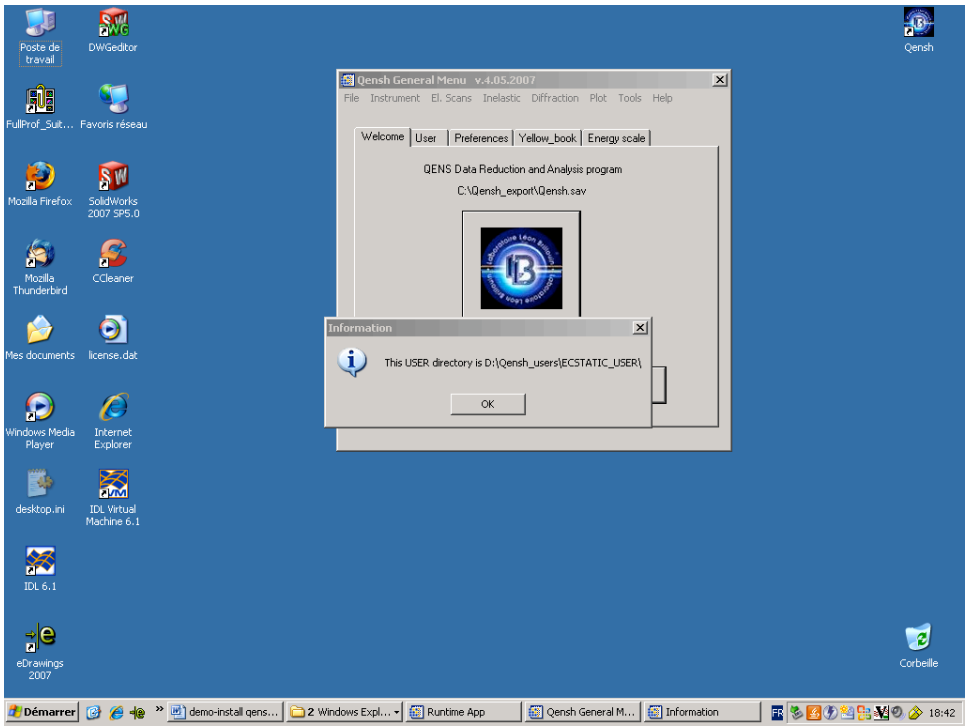
1) **Definition of a user** (in TAB User)



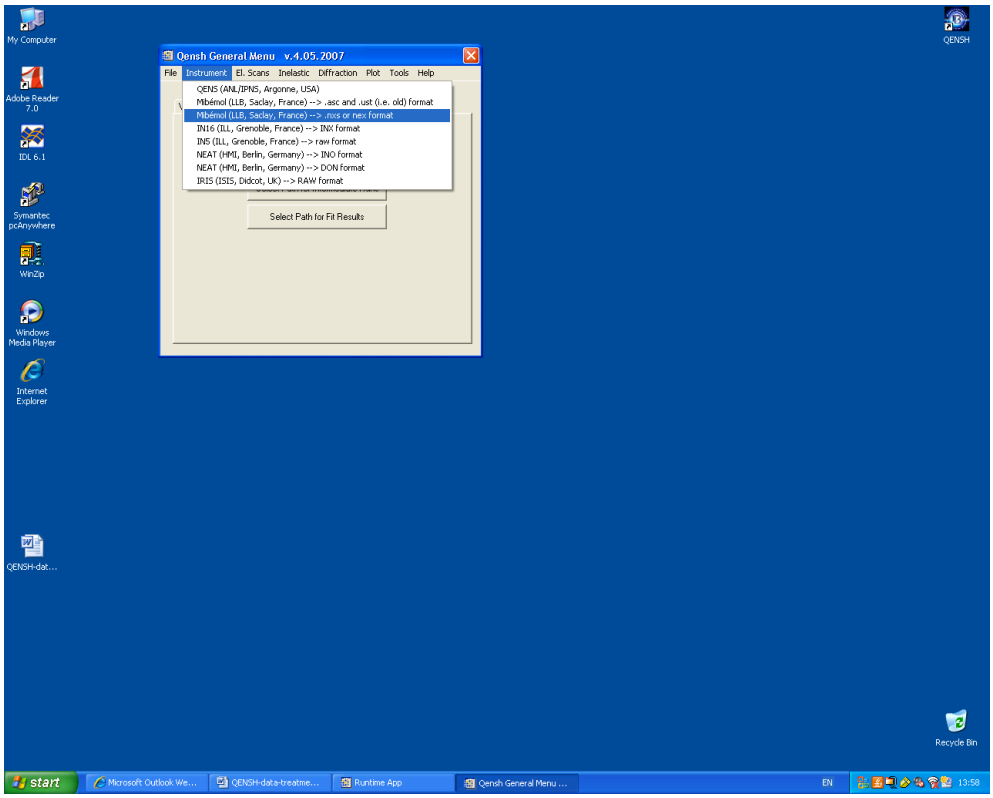
- Select 'New user' TAB and write down a new name (NOTE: no spaces in the name)
- Press Enter



- 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



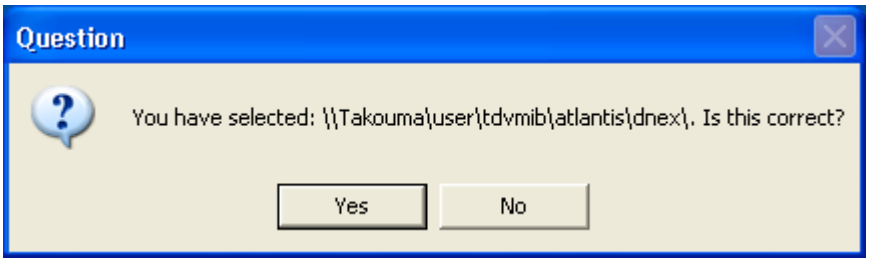
2) **Definition of instrument**



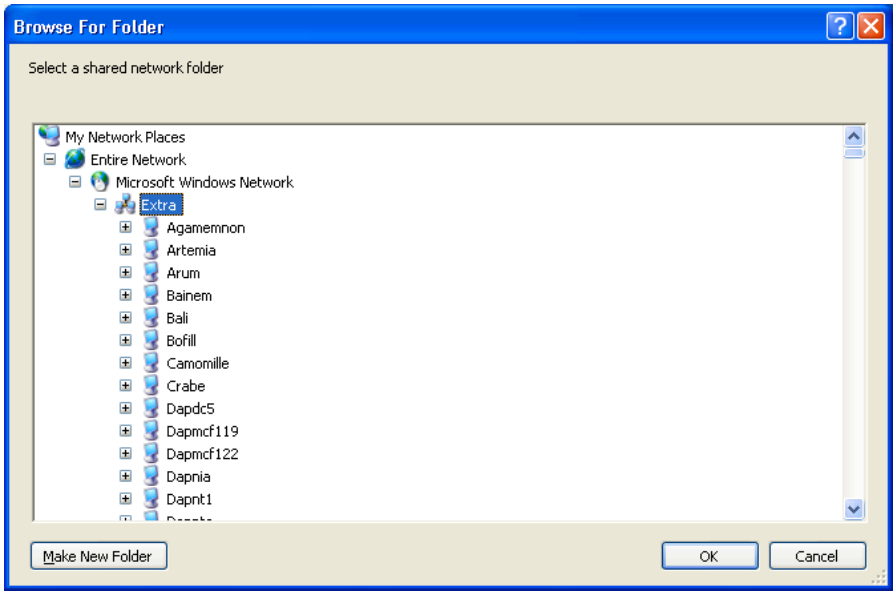
- Going to TAB Instrument – choose the appropriate instrument, all of the current data acquired on MIBEMOL are .nxs and .nex format

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

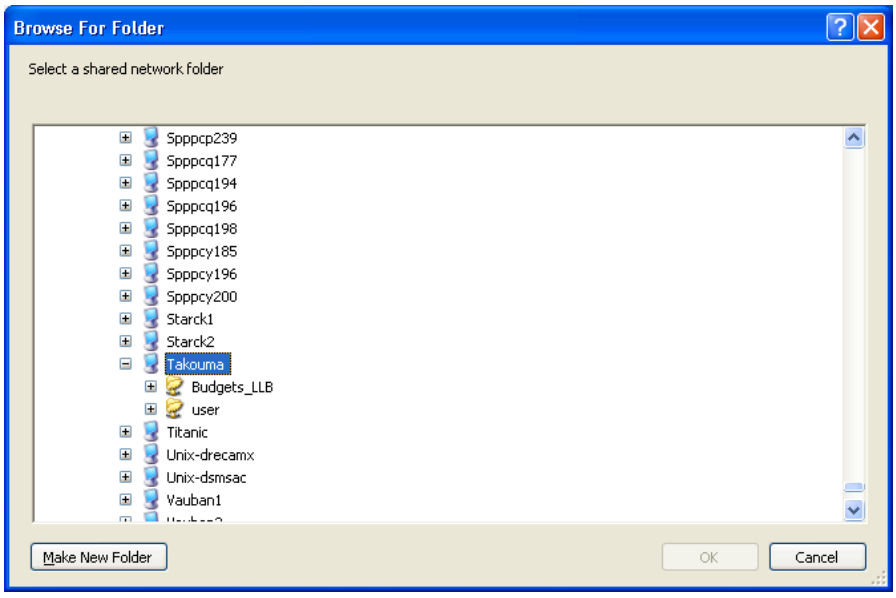
a) click on '**Select path for raw data'** and select a path



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



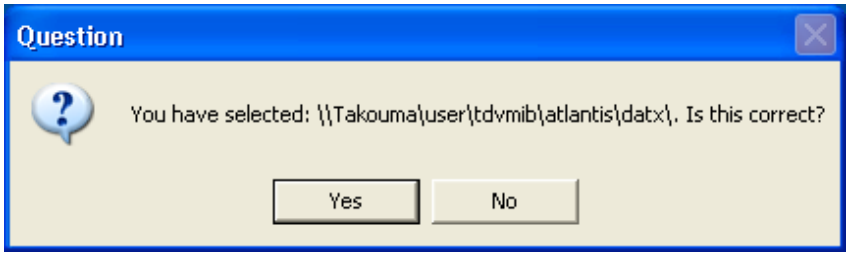
- Then scroll down to find ‘takouma’ and continue to select ‘user’ etc.



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’**

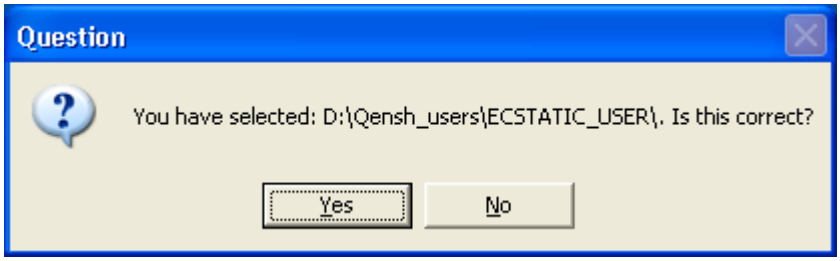
Again, when working in LLB the path to intermediate runs is:



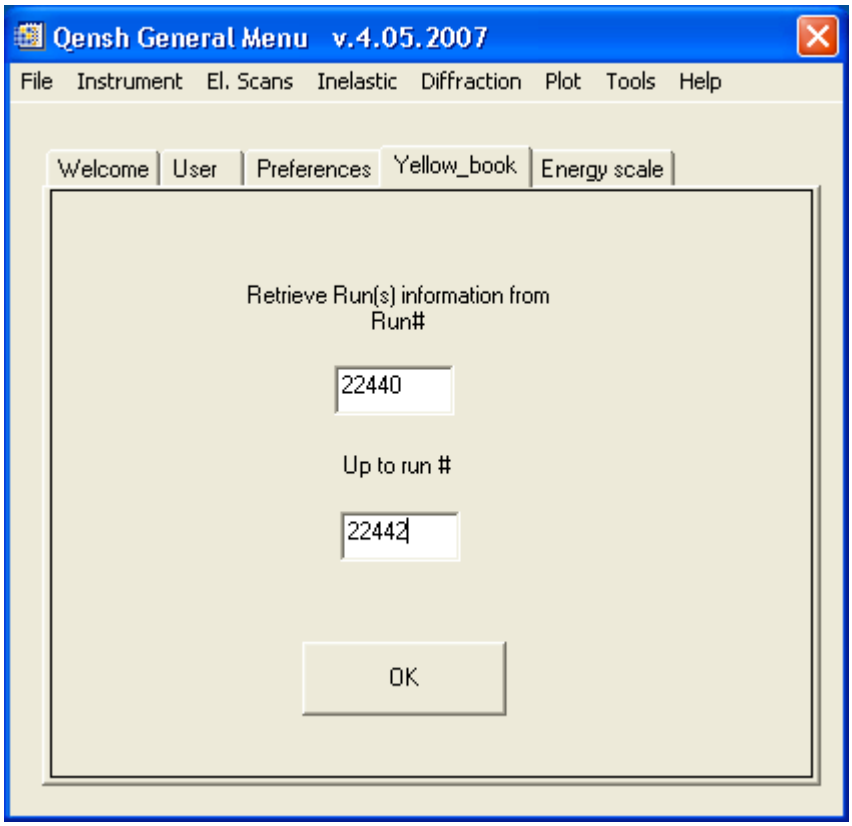
The intermediate files are called .nxs1, .nxs2 etc…

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

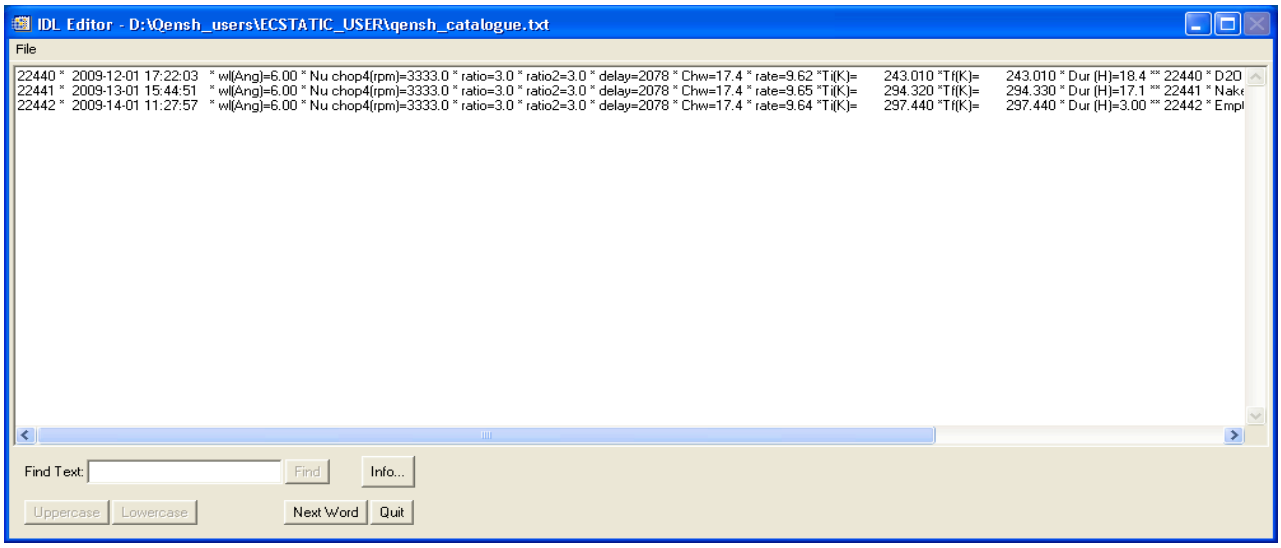
You should put the fit results in the user directory defined previously, i.e.:



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



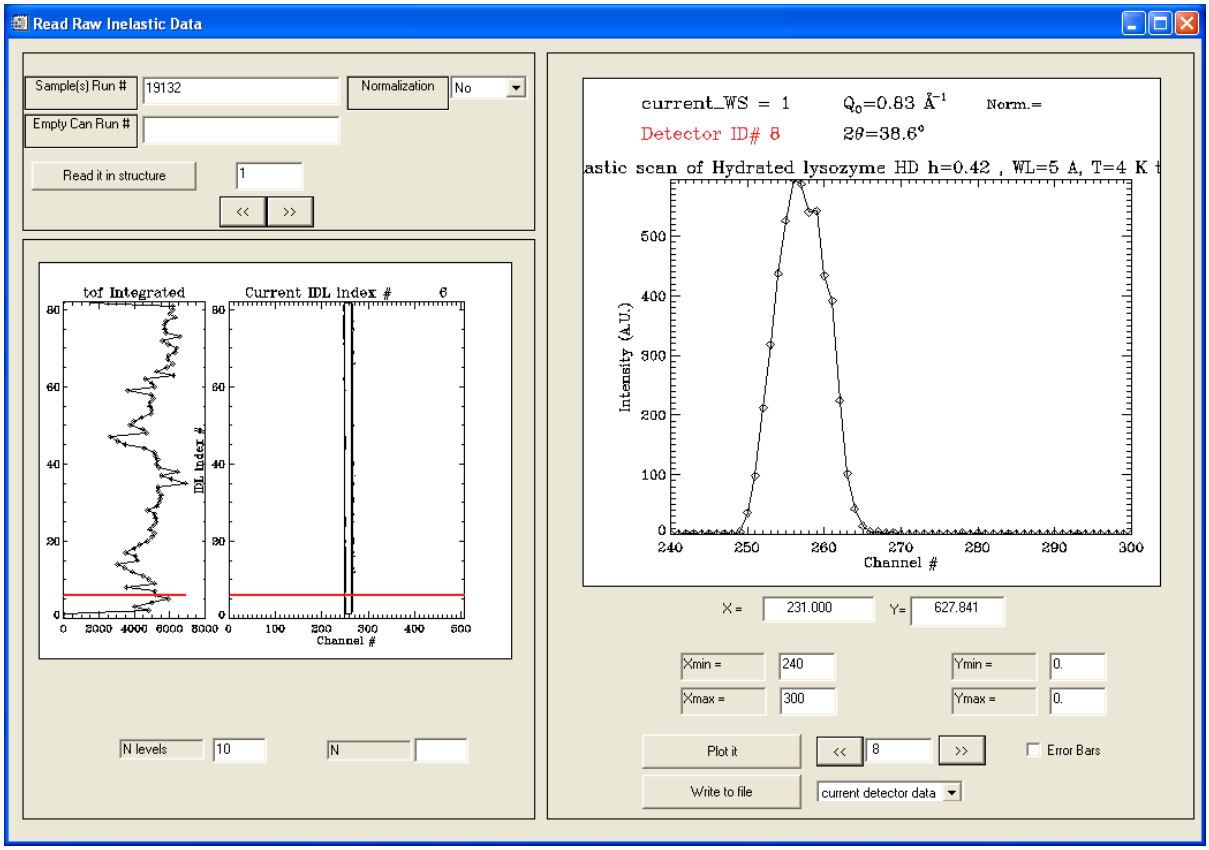
- Go to the TAB 'Yellow_book' and enter the range of run numbers to be viewed, then click on OK, the following table with details shall appear. It contains the run number, date, wavelength, some chopper settings, temperature, duration and run title:



- Click on ‘Quit’ to close the table.

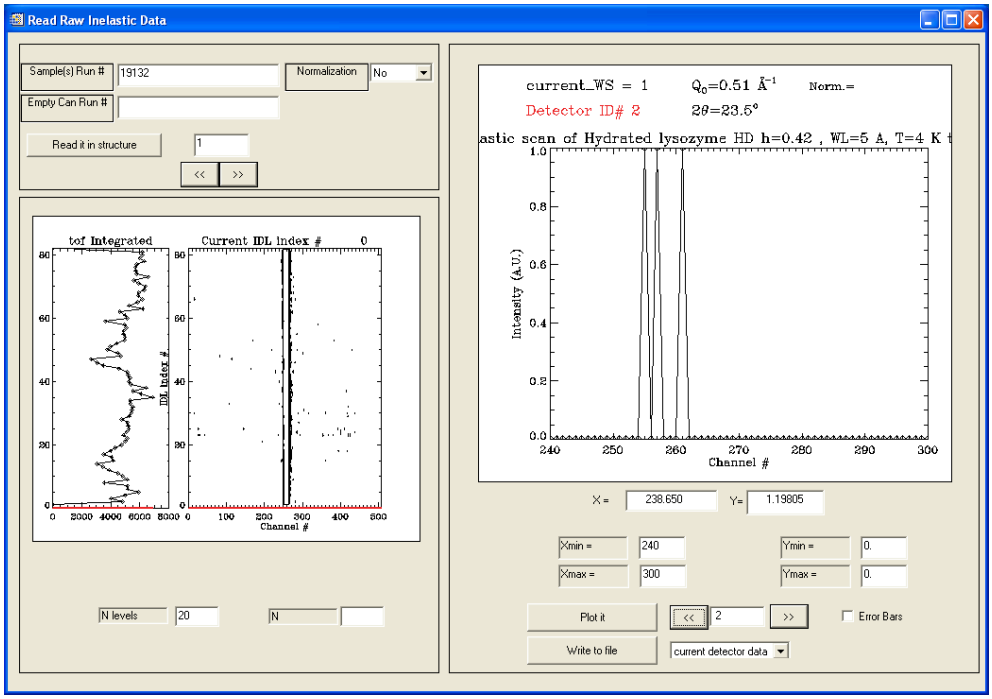
3) **Read raw data, in time-of-flight** (in TAB Inelastic)

This allows you to read the raw data (in time-of-flight), detector by detector and decide which detectors to eliminate in the subsequent “Data Normalisation and Grouping” step.



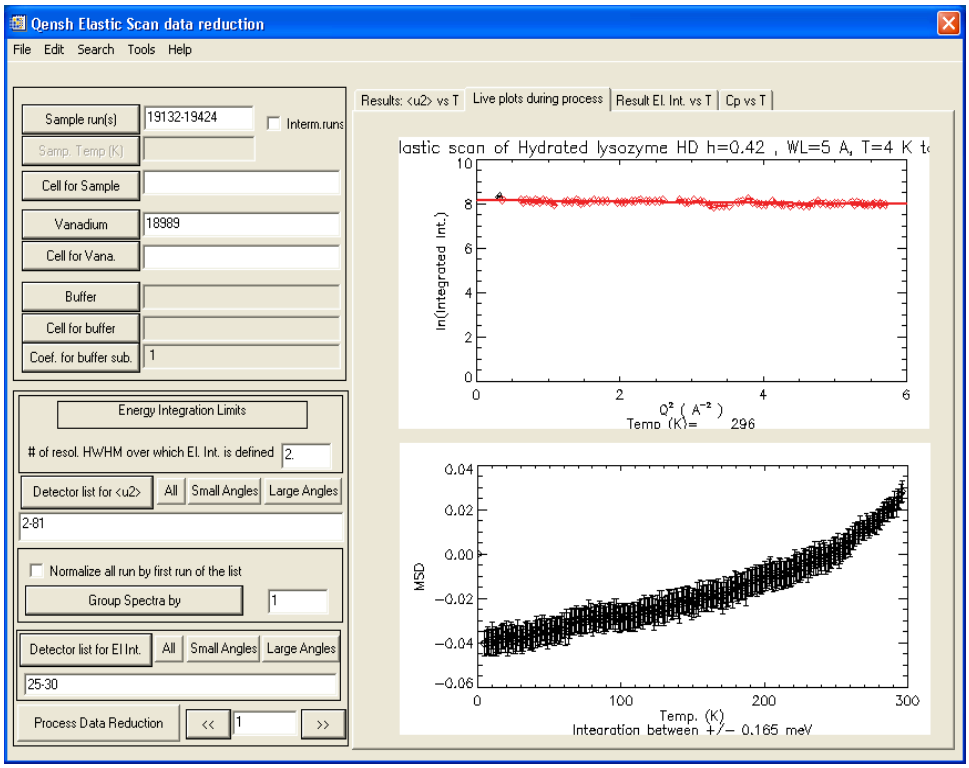
- Enter a Sample Run and press “Read it in structure”. On the left you see an integrated TOF signal as a function of angle, as well as the full TOF signal for the different TOF channels. On the right you see the TOF signal for a single chosen detector, with its ID number in red.

- On the left, by changing the value of "N levels" you change the resolution of the neutron count.
- The red line on the left image indicates the angle (i.e. the detector) that you see in detail on the right image. You can double click on the left image to change the position of the red line and thus the chosen detector. You can also scroll across the detectors by pressing the double arrows below the right image. Note that Detector No 1 does not exist for MIBEMOL, it is the place of the MONITOR. So the detectors are numbered beginning from 2.
- Any detector that shows abnormal signal (i.e. a double peak or not peak at all) has to be noted down and excluded in the "Data Normalisation and Grouping" step. Below is the example of detector No.2 of MIBEMOL, usually to be discarded:



4) **Elastic Scans** (in TAB El. Scans)

Elastic scans are usually carried out as a first test on a sample. We record, in short runs, the scattered intensity as a function of temperature. Instead of analyzing in detail the quasi-elastic broadening, we simply integrate the scattered intensity across the elastic region and look for any decrease in this integrated elastic intensity as a function of temperature. Any such decrease indicates that some scattered intensity is beyond the elastic region, i.e. in the quasi-elastic (or inelastic) region, which in itself indicates the onset of a particular type of motion.



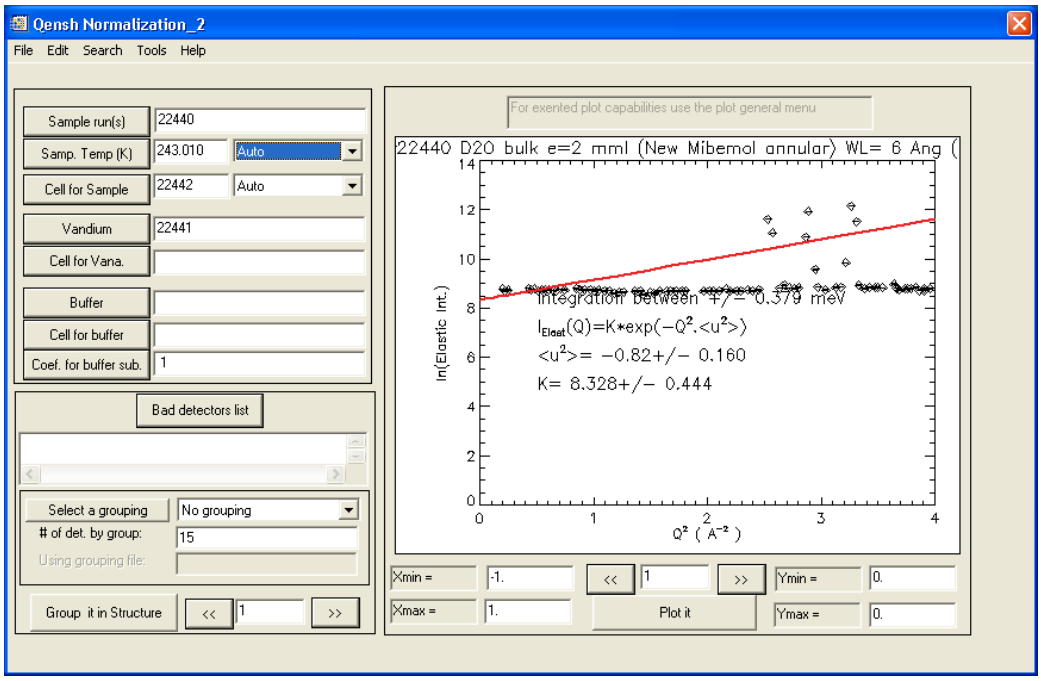
- Above: In the Elastic Scan window, specify the run numbers corresponding to the sample, can of sample, vanadium, can of vanadium (if any). It is advisable to try without the run numbers of the two cans, to see the effect they have on the data. Vanadium is used here to normalise the intensities and thus correct for different efficiencies of detectors.
- The acceptable separators for run numbers are "-" and ",". For example, if we have the runs 22441, 22442, 22443 and 22449 for the sample, we enter: 22441-22443, 22449. For more information about the correct syntax, hold your mouse over the “Sample run(s)” button, a yellow information box comes up. For the moment, DO NOT USE the option “Interm.runs”.
- Further, you specify the number of HWHM of the resolution function over which the integration of the scattered intensity is to be carried out.
- You can select only a certain region of detectors over which the analysis is to be carried out, there are two types of analysis. For each temperature you obtain:
    - a) $\langle u^2 \rangle$ (mean square displacement - MSD, related to vibrational amplitude), which is the slope of a linear fit of the logarithm of the integrated elastic intensity versus Q^2.
    - b) the sum of the integrated elastic intensities across the detectors specified (this is useful for tracing the evolution of the intensity of a Bragg peak, for example)
- If you wish to use all detectors for the two types of analysis, leave the fields below “Detector list for $\langle u^2 \rangle$” and “Detector list for El. Int” empty. Otherwise, define a detector range, e.g. 2-30.
- Ticking the option “Normalise all runs by first run of the list”, you normalise the integrated elastic intensities at a given temperature by those of the first run. By definition, the MSD of the first run is thus equal to zero, and the MSD of all consecutive runs is a kind of MSD relative to the first run – one has to be careful with the interpretation of such MSD.
- You can group spectra by inserting a value greater than 1 into “Group Spectra by”.

- At the bottom, choose a workspace and press “Process Data Reduction” to carry out the analysis. Several plots on the RHS shall appear.
- The plots on the RHS are in 4 TABS. The first TAB gives you $\langle u^2 \rangle$ versus temperature, it is identical to the bottom graph of the TAB “Live plots…”. The top graph of the TAB “Live plots …” is a plot of the Integrated Elastic intensity versus Q2 for the last run that you specified. You can see which detectors you are using for the MSD analysis – the corresponding data points appear in red, as opposed to black. The TAB “Result El. It vs T” is the integrated elastic intensity versus temperature. The last TAB gives you the heat capacity (cp) versus temperature.

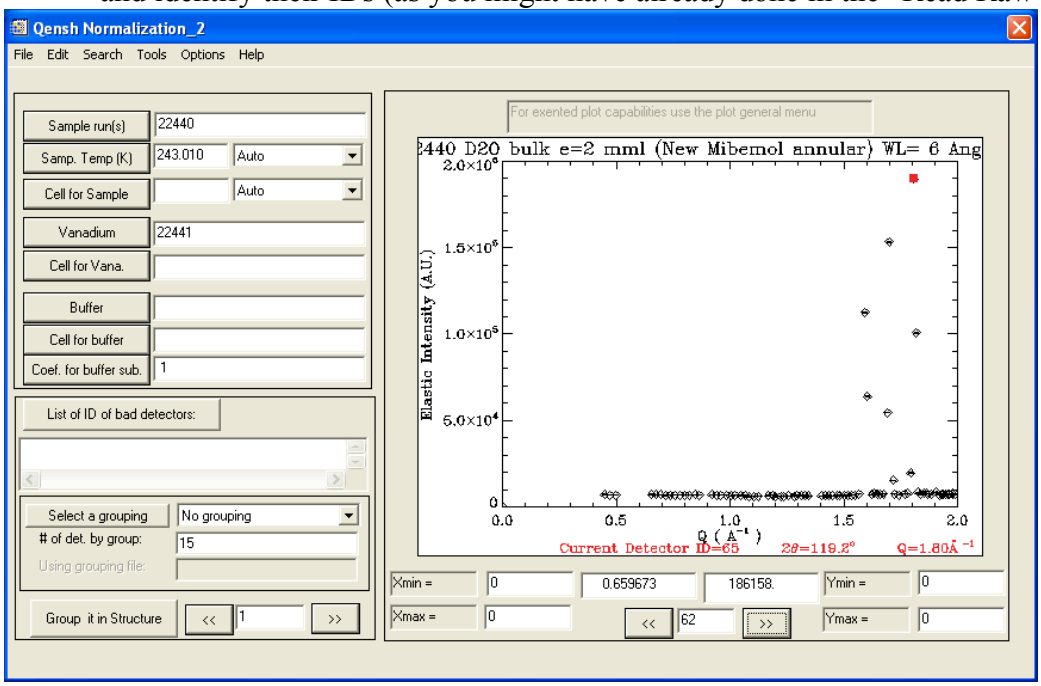
5) **Data Normalisation and Grouping** (in TAB Inelastic)

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)

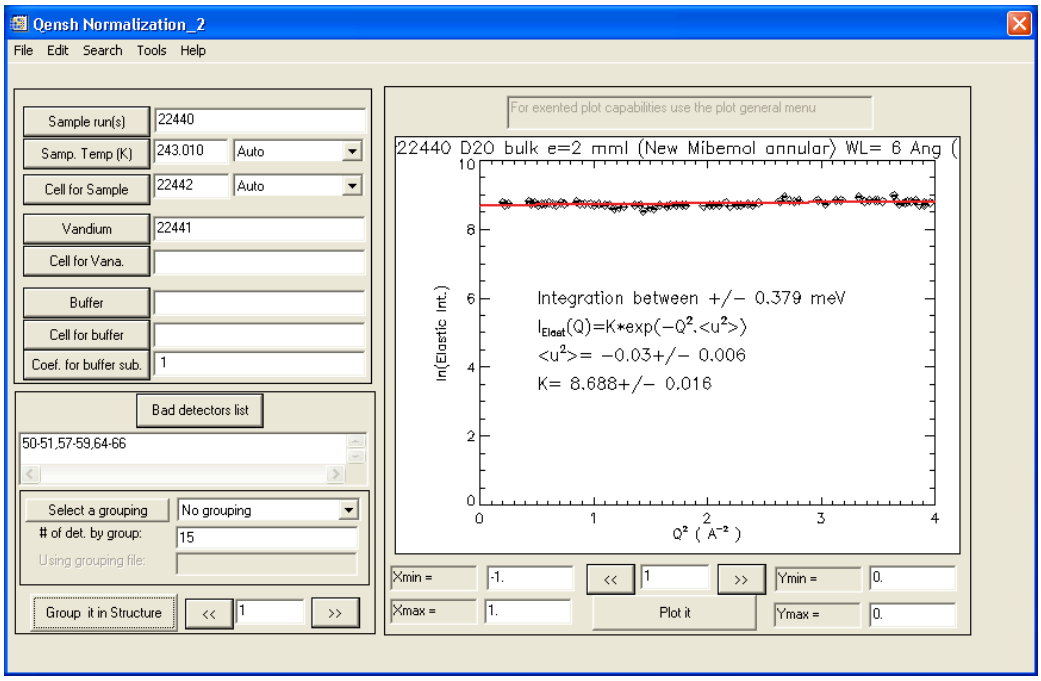
- The acceptable separators for run numbers are "-" and ",". For example, if we have the runs 22441, 22442, 22443 and 22449 for the sample, we enter: 22441-22443, 22449. For more information about the correct syntax, hold your mouse over the “Sample run(s)” button, a yellow information box comes up. Note that it is possible to chose only some subruns of a run, using e.g. 22442(1:6;8), which excludes the subrun 7 of run 22442.
- The buffer corresponds to a background sample that we might wish to subtract from the sample of interest. For example, when studying water dynamics in a hydrated clay, the buffer would be the signal from the dry clay, i.e. no water present.
- The coefficient for buffer subtraction: Using the above example, in the simplest case, we assume that the scattering from 1g of dry clay (i.e. the clay crystallites) is the same as the scattering from 1g of clay crystallites in the hydrated clay sample. In this case, the buffer coefficient would be just the ratio of the mass of clay crystallites in the hydrated clay and the mass of the dry clay sample (contains only clay crystallites). When the buffer and the sample of interest are of a different composition (i.e. a different deuteration level), then the calculation has to contain the ratios of their scattering cross-sections. Rigorously, the calculation should also include the different transmissions of the buffer and the sample of interest.
- You can subtract a buffer with a give subtraction coefficient at this stage, however it is wiser not to. Deal first the data of the sample itself (including the buffer), separately the buffer by itself. The subtractions rarely work perfectly, you can always subtract the buffer at a later stage or even include it at the stage of the fitting procedure.
- 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:



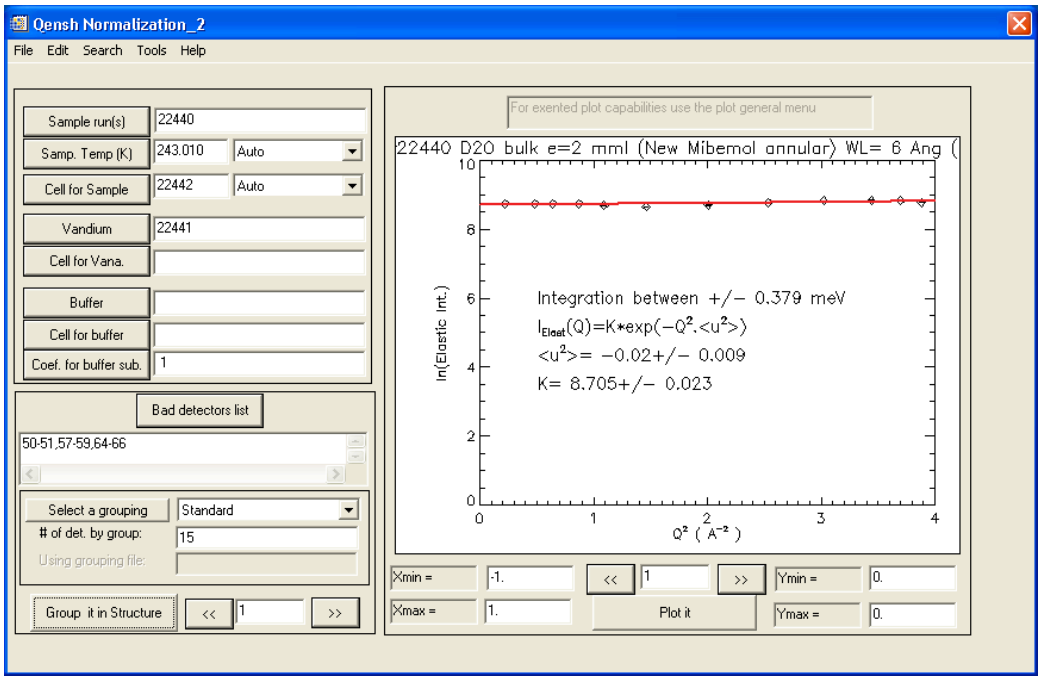
- If clear Bragg peaks appear, remove data by inserting numbers of Bad detectors (e.g. 10,11 etc). Click on the double arrows beneath the plot to scroll across the detectors and identify their IDs (as you might have already done in the "Read Raw Data" step):



- In the above 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:

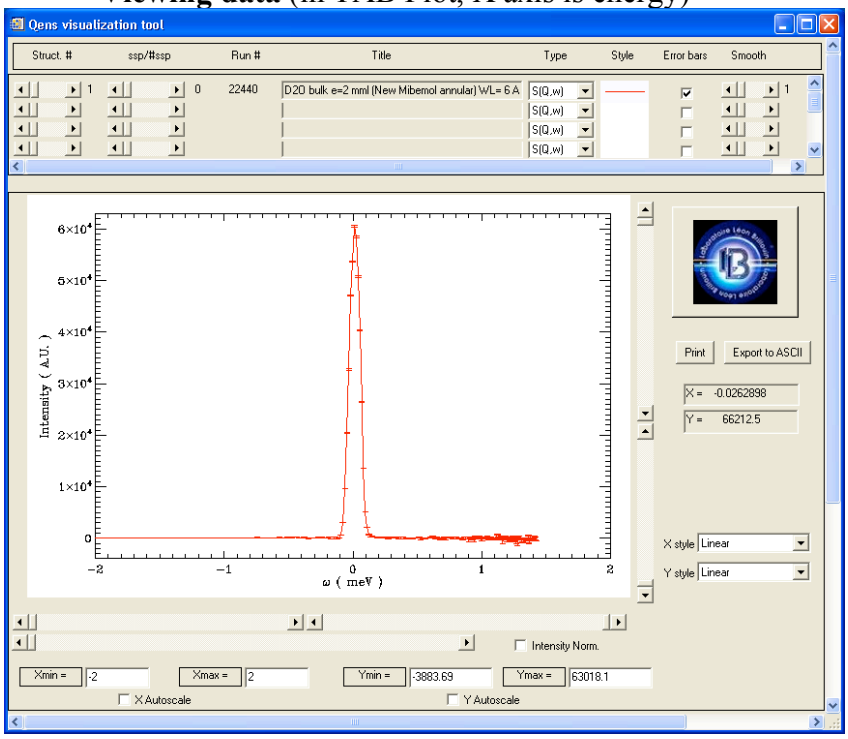


- In the above treatment for sample, vanadium is used to normalise the intensities and thus correct for different efficiencies of detectors. Grouped Vanadium signal by itself shall be used later in the fitting procedure to provide the elastic peak.
- Plot that appears on the RHS: Logarithm of the scattered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

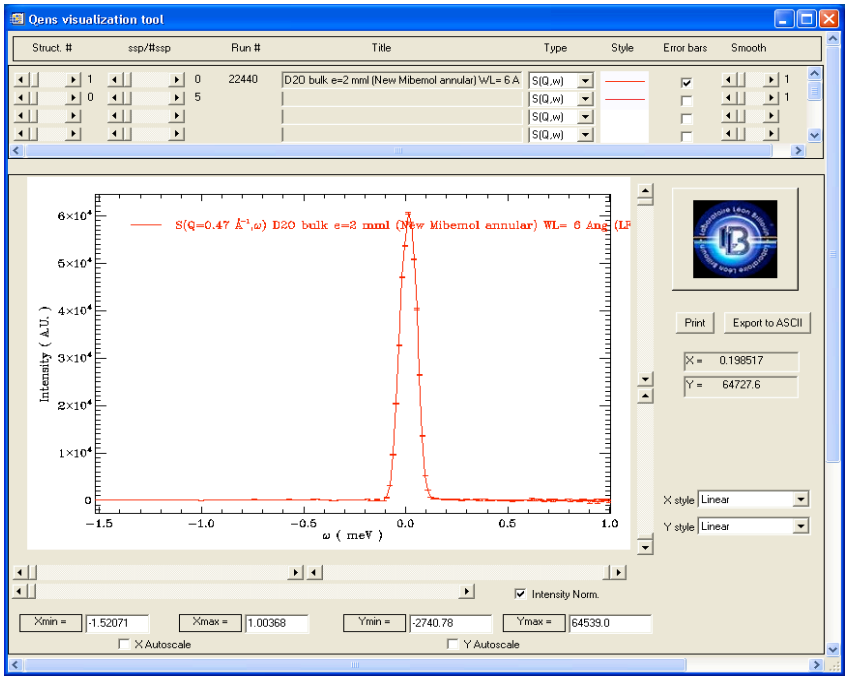
  $\langle u^2 \rangle$: slope (related to vibrational amplitude)

  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.

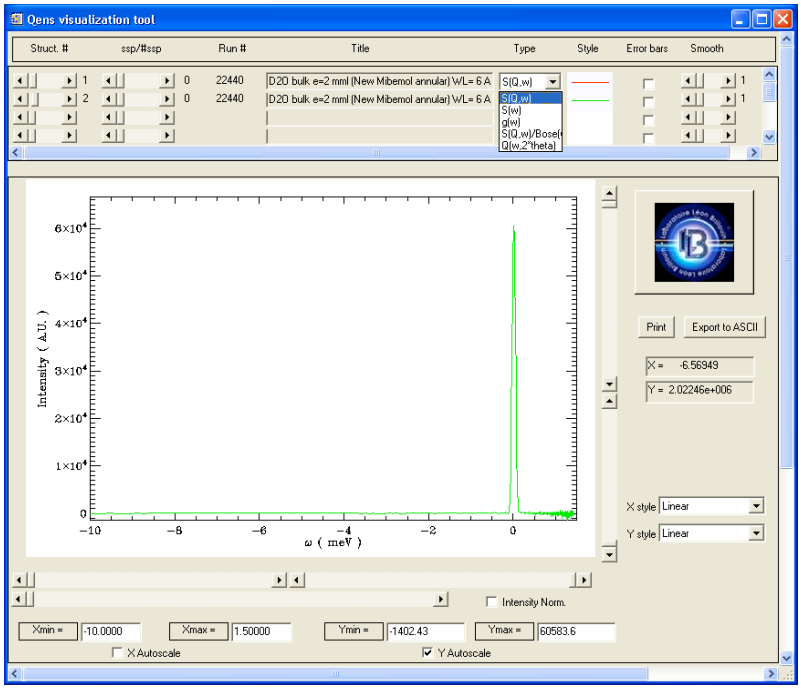
6) **Viewing data** (in TAB Plot, X axis is energy)



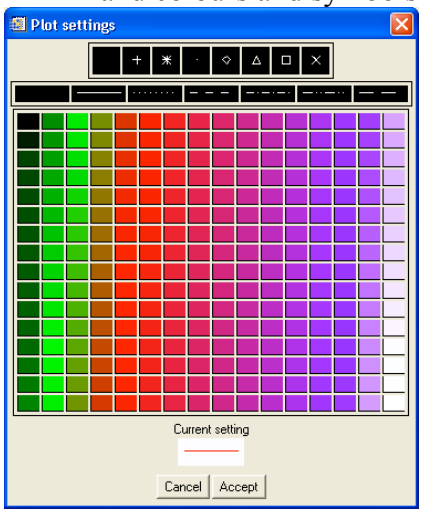
- Scroll on the 'Struct' to find the workspace desired (maximum 20 workspaces)
- Selecting the 'Error Bars' option allows the visualisation of error bars for individual experimental data points.
- Selecting 'Intensity Normalisation' below the graph window: all the graphs in the window shall be normalised 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':



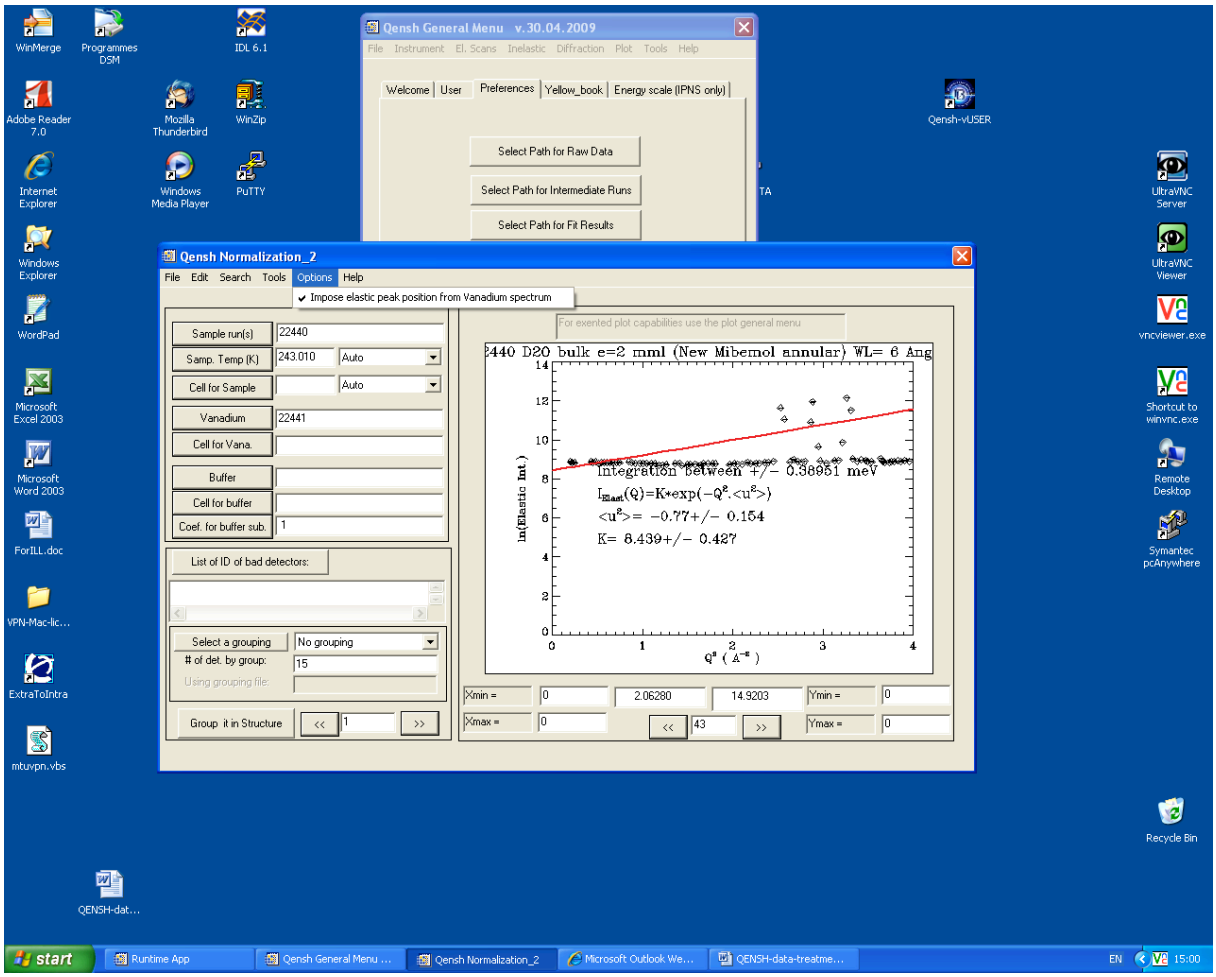
- Double clicking on the 'Style' for a given Workspace, brings up the following menu and colours and symbols can be changed (click on Accept 2times):



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.

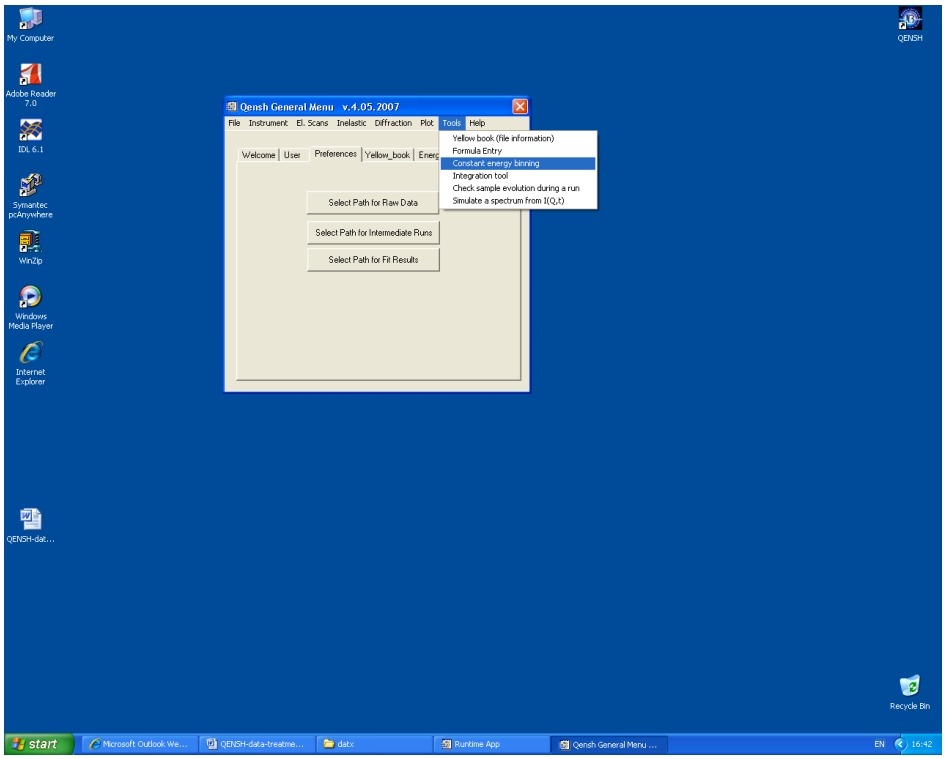
- **Problem of elastic peak from sample and Vanadium being shifted in energy with respect to each other:** this is a consequence of the sample/vanadium not being centred properly inside the sample well. This modifies the distance sample-detector and thus the position of the elastic peak. If you observe this you need to redo the step of "Data Normalisation and

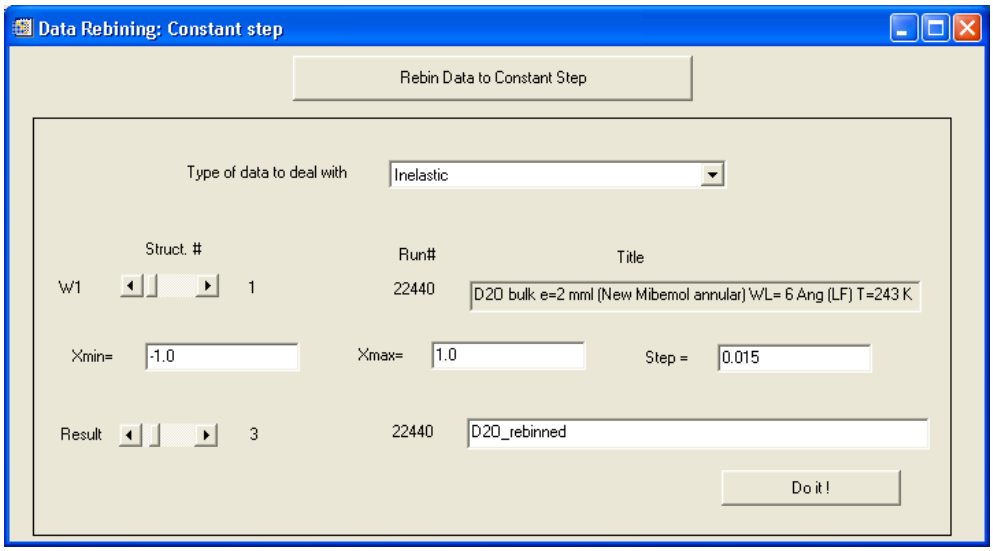
Grouping" again with the Option "Impose elastic peak position from Vanadium spectrum" being ticked:



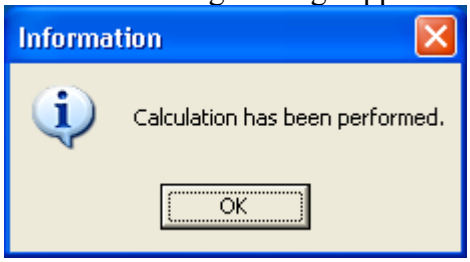
7) **Constant energy binning** (in TAB Tools)

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.

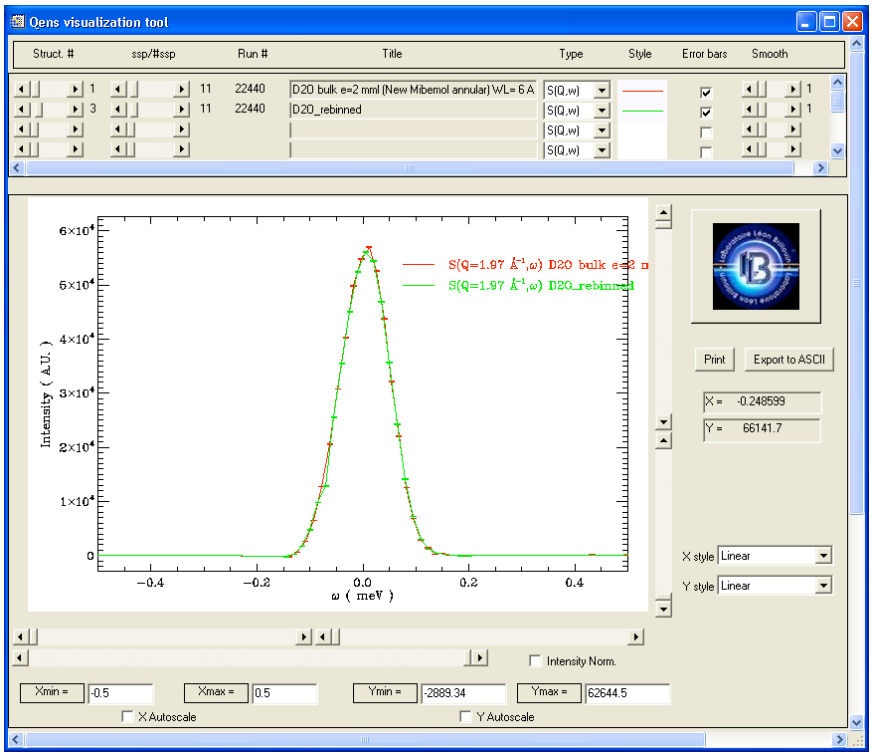




- Select type: Inelastic
- Enter the max, min, step determined previously (this is in units of meV) NOTE that the maximum number of points possible is 1800. An error message appears if you go over that number.
- Choose a NEW workspace (i.e. do NOT overwrite the unbinned data) for binned data and insert a name for the rebinned data in the window provided. When carried out the following message appears.



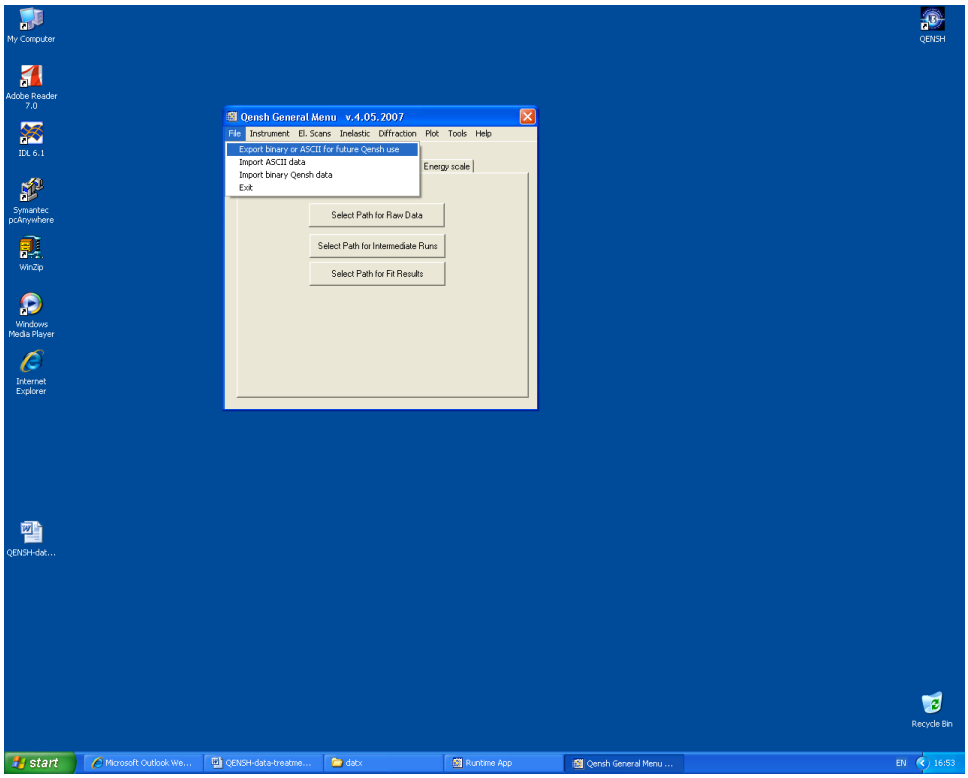
Need to do binning for both SAMPLE and VANADIUM. At the end of rebinning you need to check that the procedure has not distorted the data. So visualise both the original and rebinned data together:

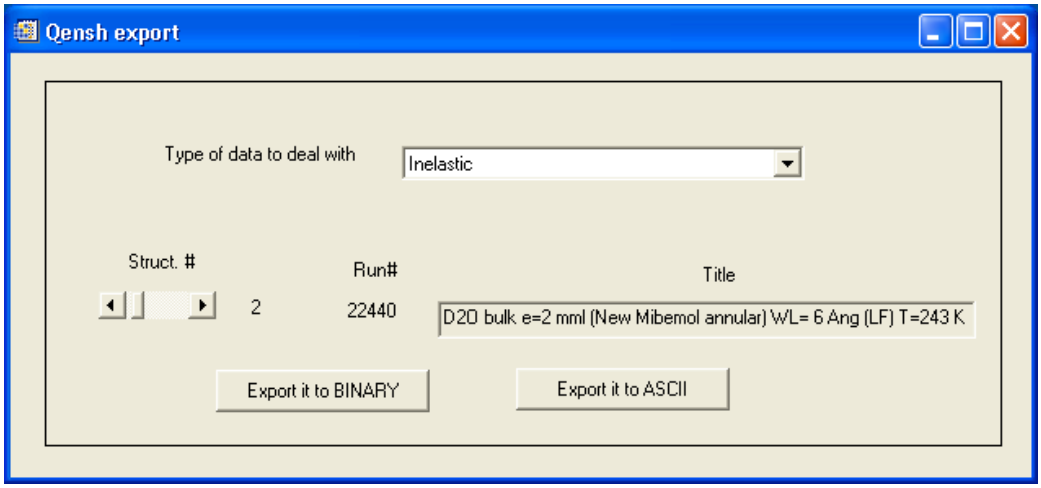


- The above shows a reasonable constant energy binning, the green and red curves are almost identical. If you are not satisfied, redo the procedure with a different rebinning step and use the same workspace for the final result to overwrite the old wrongly rebinned data.

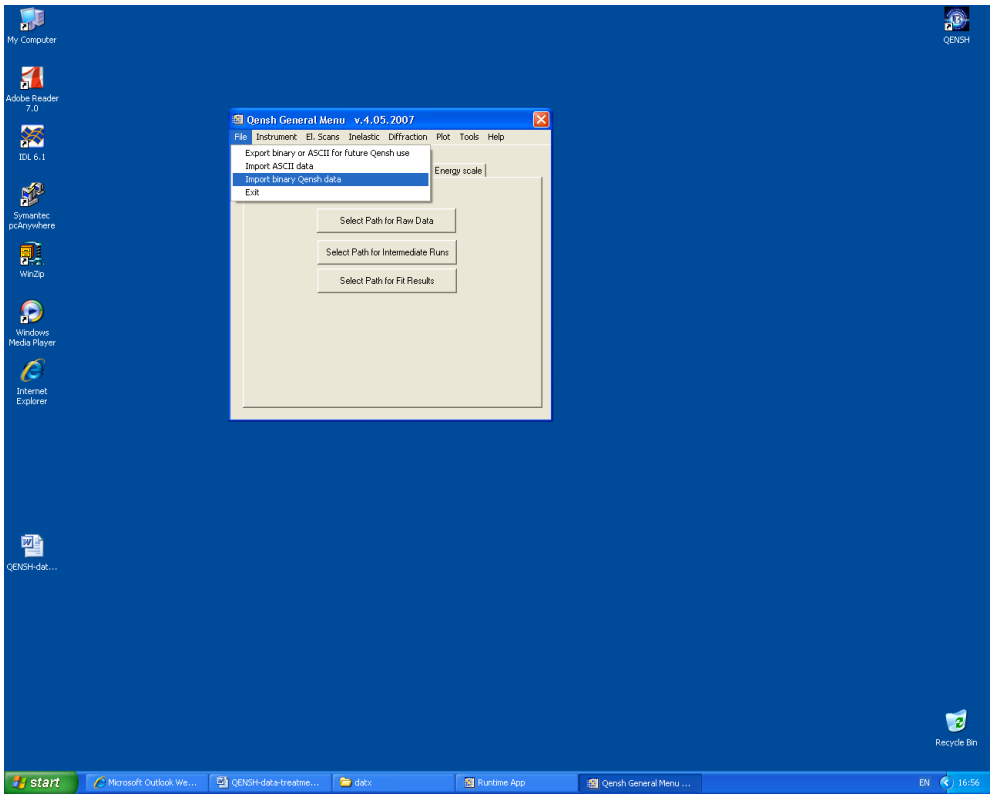
8) **Exporting binned data for future fitting** (TAB File; Export ../Import..)

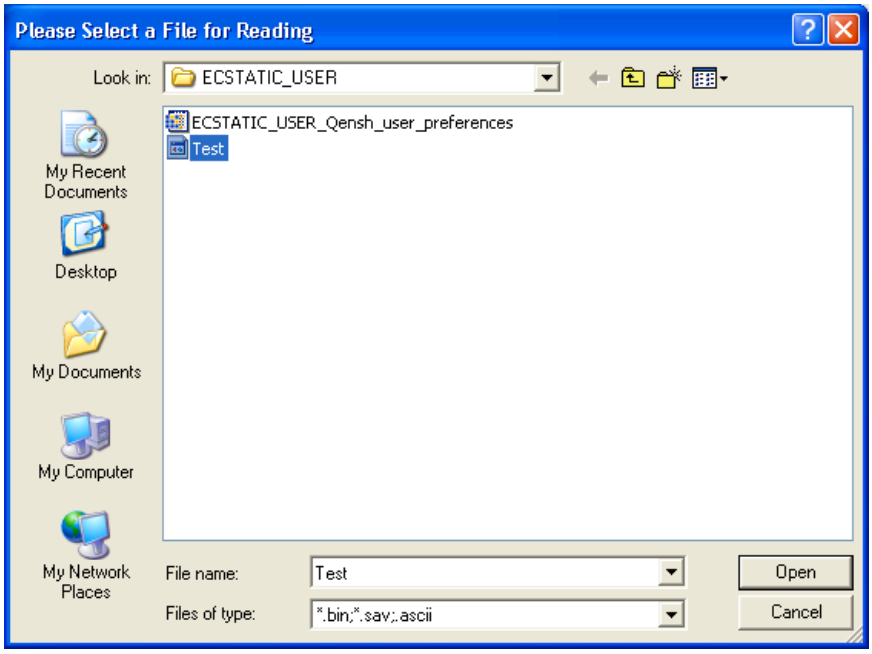
In order not to have to repeat the procedures of data normalisation and constant energy binning every times Qensh is launched, the normalised and energy binned data (both sample and vanadium) can be exported into a binary file, that can later be imported and fitting carried out directly afterwards.



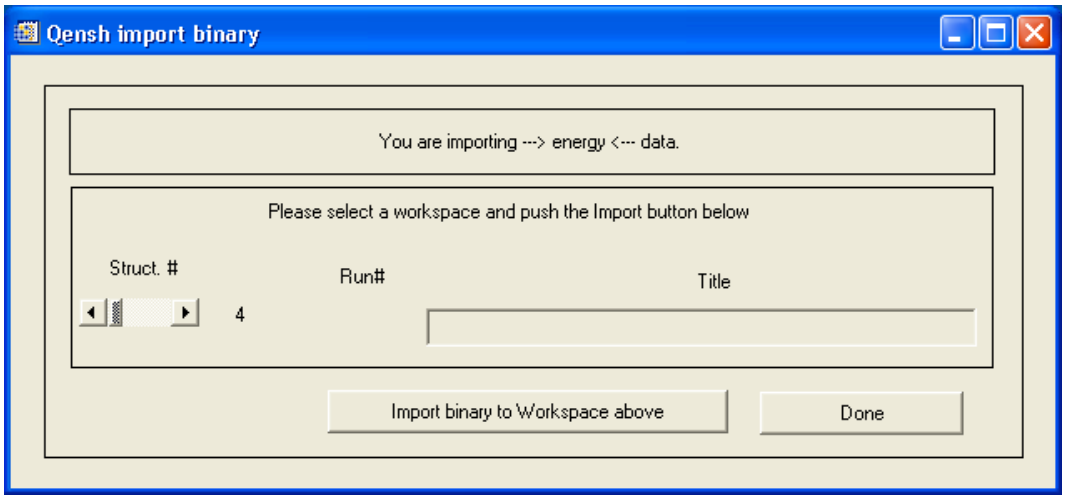


- Type: Inelastic
- Scroll to the workspace desired (NOTE the name CANNOT be changed at this stage) and click on ‘Export to BINARY’
- To Import data at a next session of Qensh:





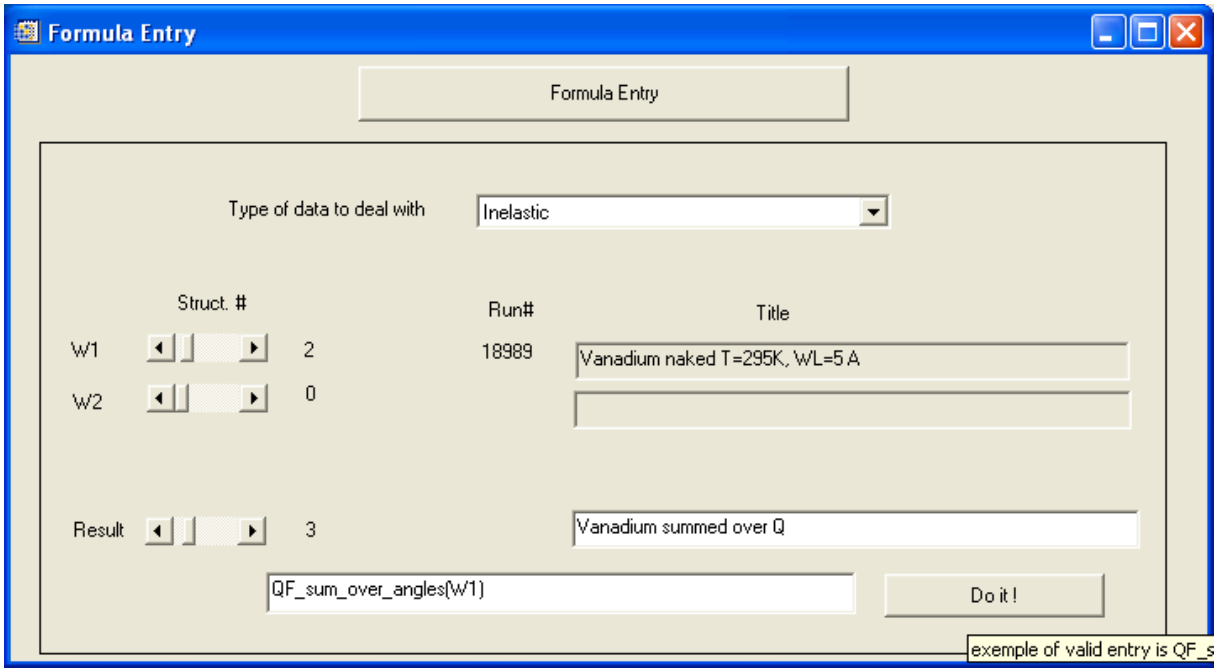
- Choose the binary file exported previously and click on Open



- Scroll to an empty Workspace and click on 'Import binary'

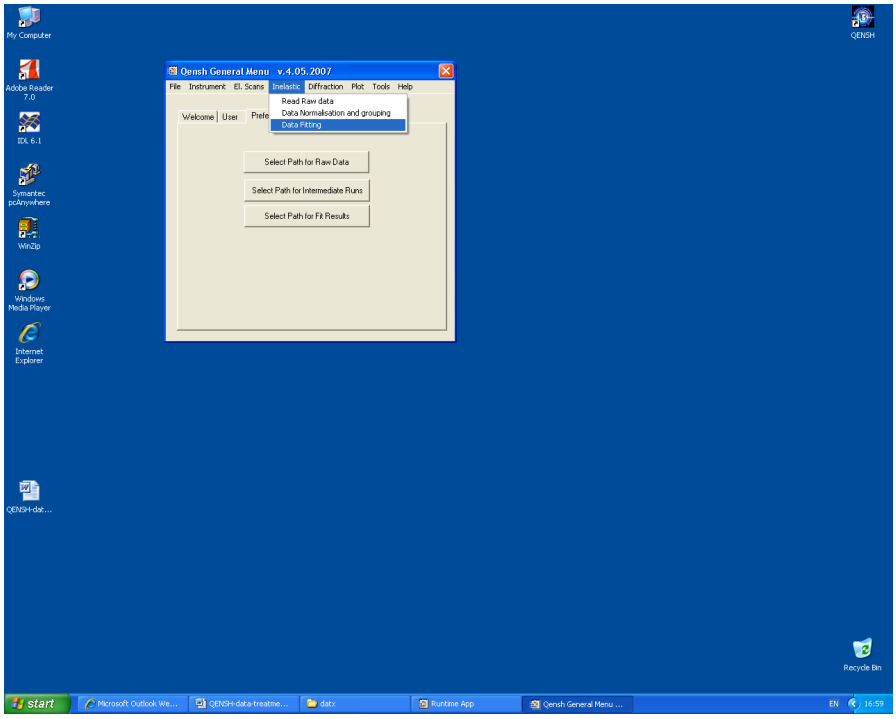
9) **Formula Entry** (TAB Tools)

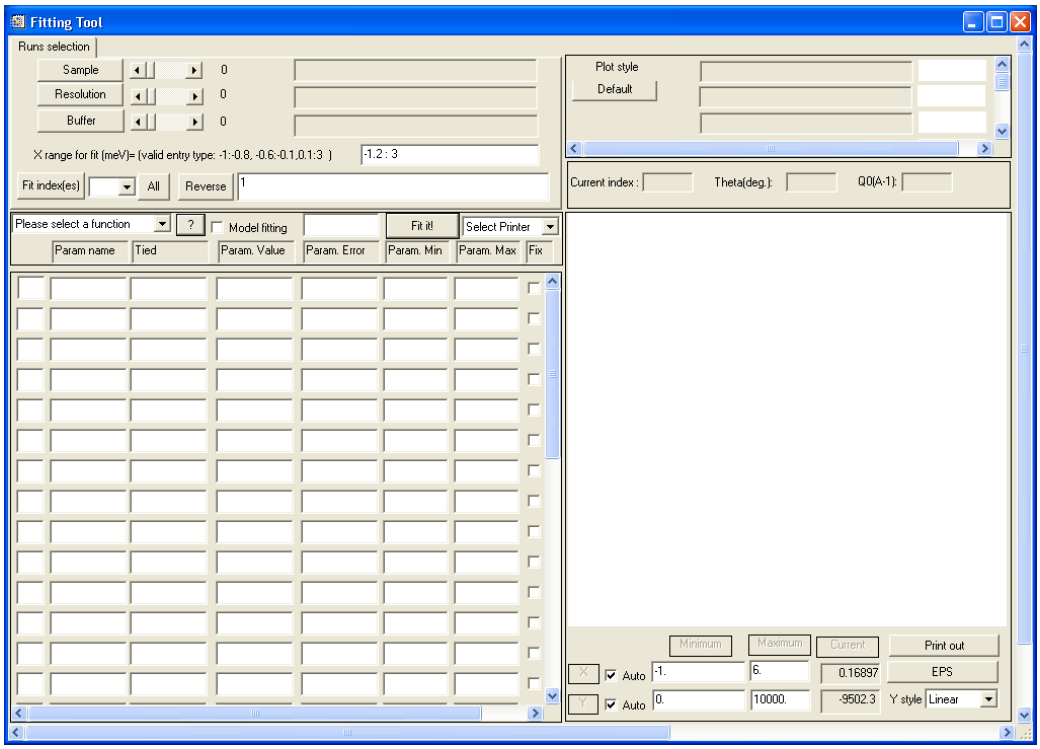
This tool allows the manipulation of runs uploaded in any two workspaces. The runs can be added, subtracted, with or without additional prefactors, i.e. W1-0.75*W2 etc. This serves for the subtraction of a buffer, for example. Some extra, more sophisticated operations also exist, you can find out about these by holding your mouse over the button "Do it" – a yellow information box comes up. One functionality is summing S(Q,w/TOF) over all Qs:



The above functionality is sometimes used for treating the signal of Vanadium when the statistics per angle is not sufficient (not counted for long enough). As the Vanadium signal is independent of Q, this makes sense.

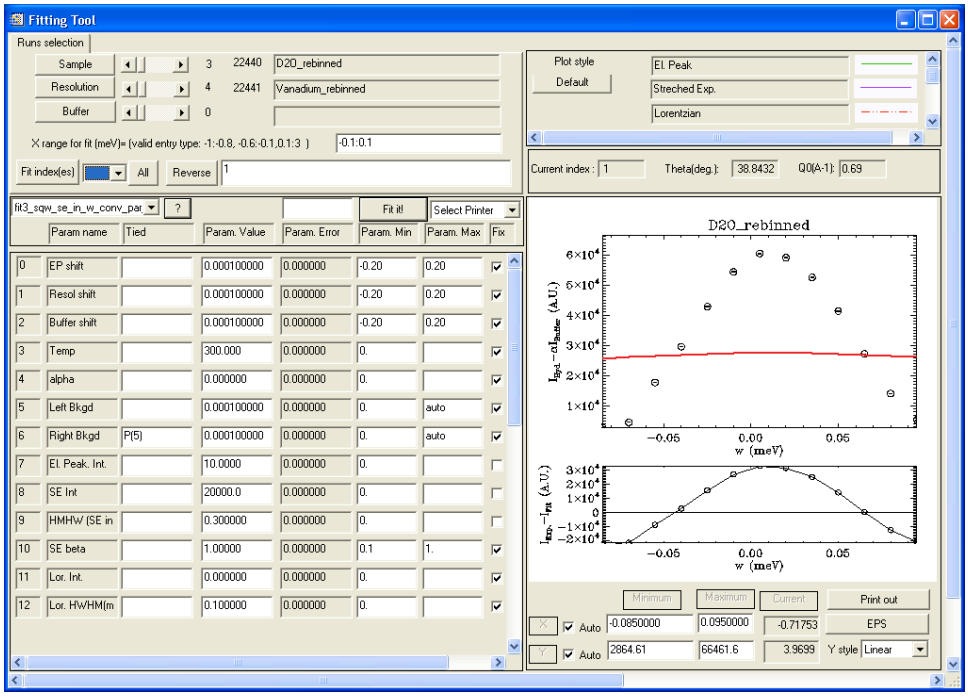
10) **Data fitting** (TAB Inelastic; Data fitting)



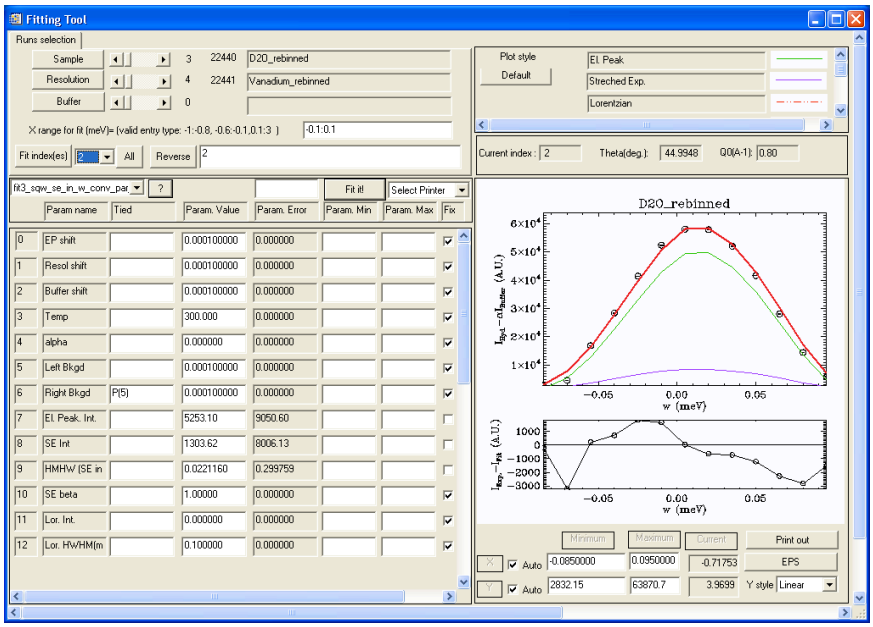


- Enter **normalized and rebinned data** for sample and vanadium (possibly buffer)
- Remember that for Vanadium, which is used in the fitting to define the width of the elastic peak, you can use the Vanadium signal summed over all Qs, if your statistics per Q is not sufficient. This of course makes no sense for the sample, as the signal for your sample is most often NOT Q-independent.
- Define x-range for fit, this has to be at most the range over which the data has been rebinned.

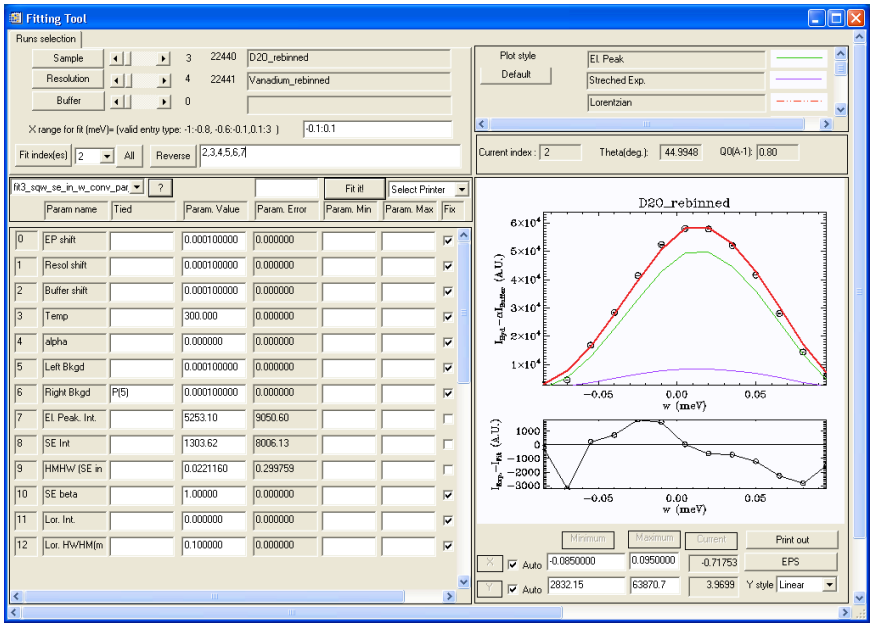
- Select a fitting function. After a fitting function is selected, to view the explanation of the fitting parameters, click on the "?" next to pull down menu of functions – a .pdf file shall open. Once a function is selected, the following appears:



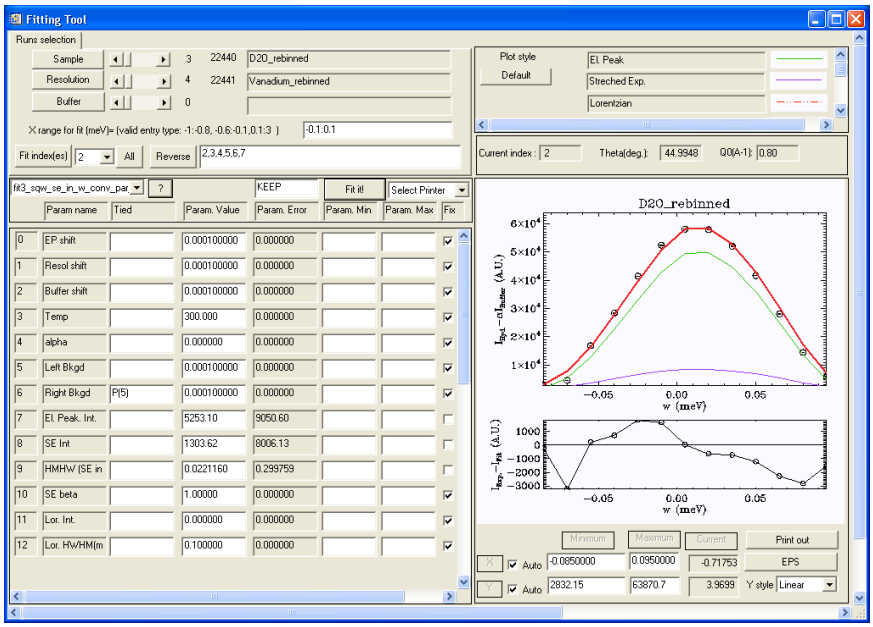
- Now choose a fit index out of the pull down menu to fit a single S(Q,w). The Q that you are fitting appears above the graph on the RHS.
- Modify the initial values for the fitting parameters. Press enter after each modification so that the new value is taken into account, the graph on the RHS changes accordingly, telling you what the modelled signal looks like with the parameter entered.
- NOTE: When you enter a number into a parameter followed by '!', the same value shall be used as the initial value for all Qs – very useful!
- 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.
- There is an option of fitting data in the **log scale**. **Three** steps need to be carried out prior to using this option:
    - In the pull down menu of the fitting function, choose the last function, the name of which ends with "fit_log"
    - In the TAB "Fitting Options", make sure that "Fit in Log" is ticked
    - In bottom RHS corner choose "Log" as the style for the Y axis of the graph.



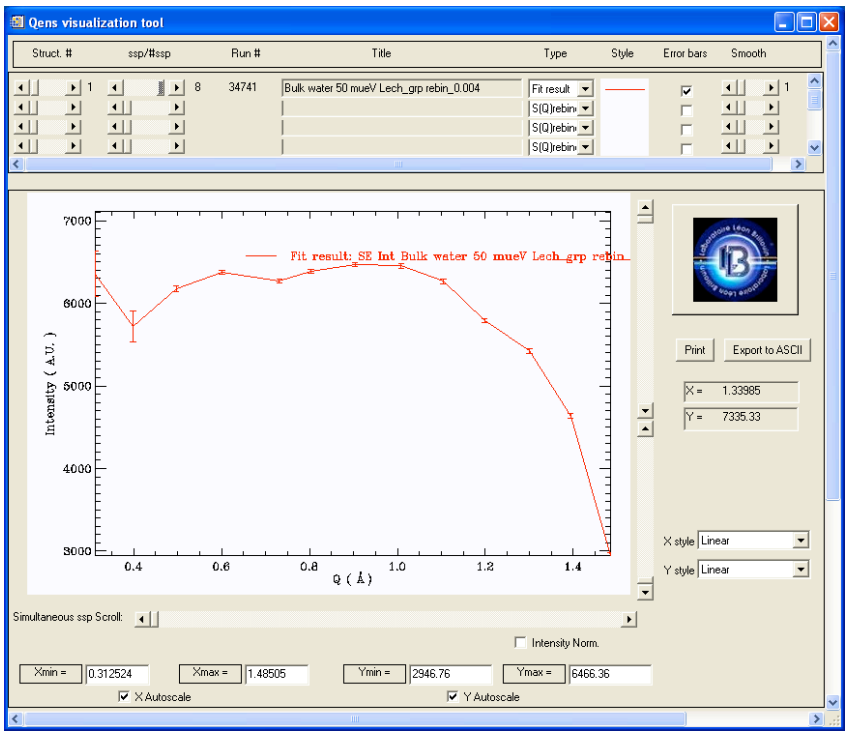
- If you wish to fix certain parameters throughout the fitting, just put in the desired value (followed by enter) and then check the box at the end ‘Fix’.
- You can tie parameters to the same value, such as is done above for the Right and Left Background, i.e. parameter 6 is tied to parameter 5, P(5).
- 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 all the experimental data points together with the resulting values of the fit (a .dat file), a figure with the final fit (a postscript file) and the final fit parameters (a .blk file).
- Most of the output files are not so useful, 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:



- Every time you change the sample or resolution file, reselect the fitting function to make sure the change in file is taken into account.
- If you fit the entire set of Q values, you can visualise the resulting set of parameters via 'Plot → x axis is Q', stay in workspace 1 and select "Fit result" as the Type to plot. The subspaces now correspond to the different fitting parameters 0-12. Double click on the figure to obtain the legend and see clearly which fitting parameter you are visualizing:



THE END