

A user manual for analyzing small angle neutron scattering data using LAMP-SANS spreadsheet (v. 1 - July 2012)

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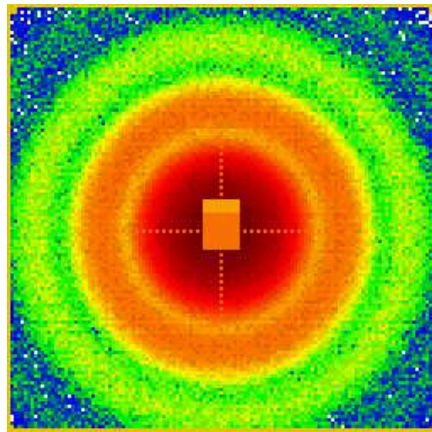


Table of contents

1. Introduction

2. Starting the interface

3. Using SANS spreadsheet

- 3.1 Select the correct instrument
- 3.2 Set the data path
- 3.3 Fill the spreadsheet
- 3.4 Check or modify the treatment options
- 3.5 Define the masks
- 3.6 Calculate the transmissions
- 3.7 Calculate the center for each configuration
- 3.8 Treat
- 3.9 Looking and manipulating the results
- 3.10 Save the table and the results

4Data treatment and corrections applied

5Anisotropic data

6Kinetic data

7D16?

8Final remarks and acknowledgments

9Appendixes

1. Introduction

SANS spreadsheet is the LAMP interface to perform the standard data reduction of a small angle neutron scattering (SANS) experiment. It has the appearance of a table to be filled by the user with the numbers corresponding to the measurements to be reduced, as well as those corresponding to the ancillary measurements required to perform the full data treatment, i.e. water calibration and direct beam, background and absorbent (Cd or B₄C) runs for each detector distance.

The present manual introduces the interface and shows the different possibilities allowed by the program. The data reduction procedure is also briefly described here, but the reader interested in getting more information about all the details related to the data reduction of SANS experiments is advised to consult some of the following references:

[1] “A computing guide for small-angle scattering experiments”; R. E. Ghosh, S. U. Egelhaaf, and A. R. Rennie, ILL technical report ILL98GH14T.

[2] “Scattering experiments: Experimental aspects, initial data reduction and absolute calibration”; Peter Lindner in “Neutrons, X-rays and Light: Scattering Methods Applied to Soft Condensed Matter”, P. Lindner and Th. Zemb (eds.), Elsevier (2002)

[3] “Small-Angle Neutron Scattering and Application in Soft Condensed Matter”; Isabelle Grillo in “Soft-Matter Characterization”, R. Borsali and R. Pecora (eds.), Springer-Verlag (2008).

[4] “Improvement of data treatment in small-angle neutron scattering”; A. Brulet, D. Lairez, A. Lapp and J.-P. Cotton, *J. Appl. Cryst.* **40**, 165-177 (2007).

[5] “Analysis of water scattering used for calibration of small-angle neutron scattering (SANS) measurements”; P. Lindner, F. Leclercq, and P. Damay, *Physica B* **291**, 152-158 (2000).

2. Starting the interface

The SANS spreadsheet can be started from LAMP either:

- 1) From the Tools menu, selecting *SANS TREATMENTS* and then *SPREADSHEET input: Grouping 1-3 configurations* (Fig. 2.1).
- 2) Or by typing directly *sans_sheet* in any of the available command lines in LAMP (Fig. 2.1)

In both cases the interface shown in Fig. 2.2 will appear and at the same time the main LAMP interface will be minimized.

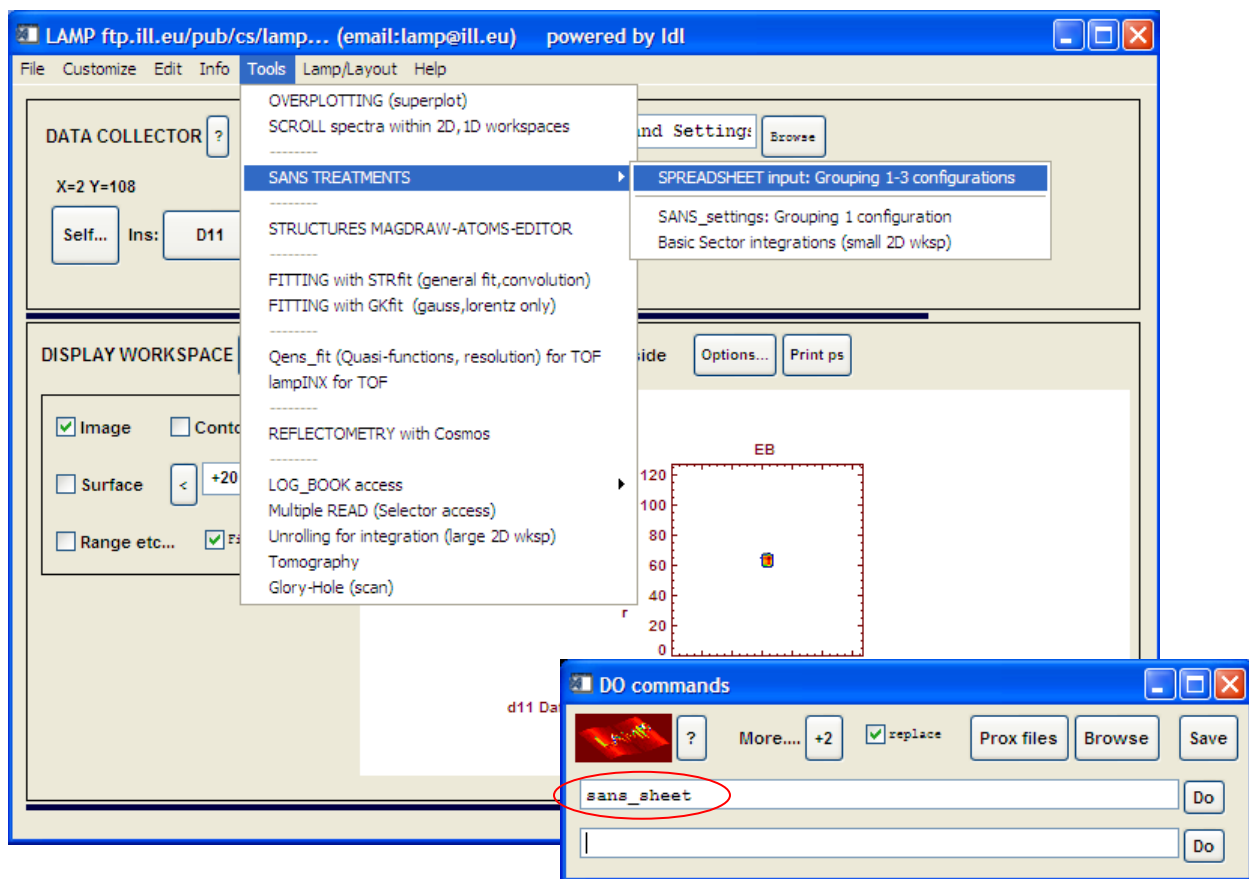


Figure 2.1: Launching the SANS spreadsheet from the Tools menu or from a command line.

Sans Inputs V1.74 (Feb 2012)

D11/Path Treatment Options Mask Transmission Center Help/Use

Cells... Samples # 90 Fill down sample incr: 1.0 Load settings Save Group: 1.00 TREAT

Data path: \\serdon\\l1data\\data\\d11\\

WATER RUNS. Notes->

	Water run	Cd/B4C run	W. cell run	Thickness Cm	Tr.Water run	Tr.Wcell run	Tr.Wbeam run
Default (High Q)				-	-	-	-

LOW ANGLE. Notes->
MIDDLE ANGLE. Notes->
HIGH ANGLE. Notes->

	LOW Q run	MIDDLE Q run	HIGH Q run	Transm. run	<-> Tr.value	-> Tr.error	-> Lo Counts
Beam Tr.					-	-	
Cd/B4C				-	-	-	
Cell Bg.							

SAMPLE inputs.

Sample IDs	LOW Q run	MIDDLE Q run	HIGH Q run	Transm. run	Thickness Cm	<-> Tr.value	-> Tr.error
S1							
S2							
S3							
S4							
S5							
S6							
S7							

Sans Inputs kirschner_June2012_static.sav V1.8 (Jul 2012)

MILAND/Path Treatment Options Mask Transmission Center Help/Use

Cells... Samples # 25 Fill down sample incr: 1.0 Load settings Save Group: 1.0 TREAT

<<.....>>

WATER RUNS. [Mask=00,00,00,00] Notes->

	Water run	Cd/B4C run	W. cell run	Thickness Cm	Tr.Water run	Tr.Wcell run	Tr.Wbe

SCAN1 ANGLE. [Mask=00,00,00,00] [Cx=Cy=00,00,00,00] Notes->
SCAN2 ANGLE. [Mask=00,00,00,00] Notes->
SCAN3 ANGLE. [Mask=00,00,00,00] Notes->

	SCAN1 Q run	Transm. run	<-> Tr.value	-> Tr.error	(((
Beam Tr.			-	-	
Cd/B4C		-	-	-	-
Cell Bg.					

SAMPLE inputs.

Sample IDs	SCAN1 Q run	Transm. run	Thickness Cm
S1			
S2			
S3			
S4			
S5			
S6			
S7			

Figure 2.2: Main interface of the SANS spreadsheet. The lower image shows the variation of the interface for D16.

3. Using SANS spreadsheet

Ideally the interface should be quite intuitive and the help item in the menu bar summarizes the main steps that the user should follow to treat the data. However we explain briefly here the basic workflow to follow when analyzing a SANS experiment.

1) Select the correct instrument:

The actual instrument selected appears on the first item of the top menu: *Instrument/Path*. If an instrument has been selected on the main LAMP interface (figure 2.1), this will be the instrument selected. Otherwise D11 will appear by default. If the selected instrument is not the desired one, it can be changed using the option '*Change Instrument Name*'. Note that this is the **first thing to do**, as changing the instrument will reset the table, so any information introduced previously will be lost. If **old data** are being treated, the user should pay attention to select the correct instrument version (e.g. D11 < 07, D11 < 98, D11 < 02), as the instrument characteristics will be different.

2) Set the data path:

Again the path to look for the raw numors will be taken from the current settings of the main LAMP interface. The user can check the actual path using the option '*Show Data path*' and the current path will be written in the space situated between the first line of the user interface and the dialog window named '*WATER RUNS*'. All the messages sent by the program will appear here. If the path is not correct, the user can change it using the option 'Set Data path' and selecting the right one using either the OS explorer or LAMP (Fig. 3.1). Finally if a calibration file exists, it can also be loaded. Note that this should be done before reading any data because the calibration is applied while reading, so otherwise it could happen that calibrated and non calibrated data are mixed.

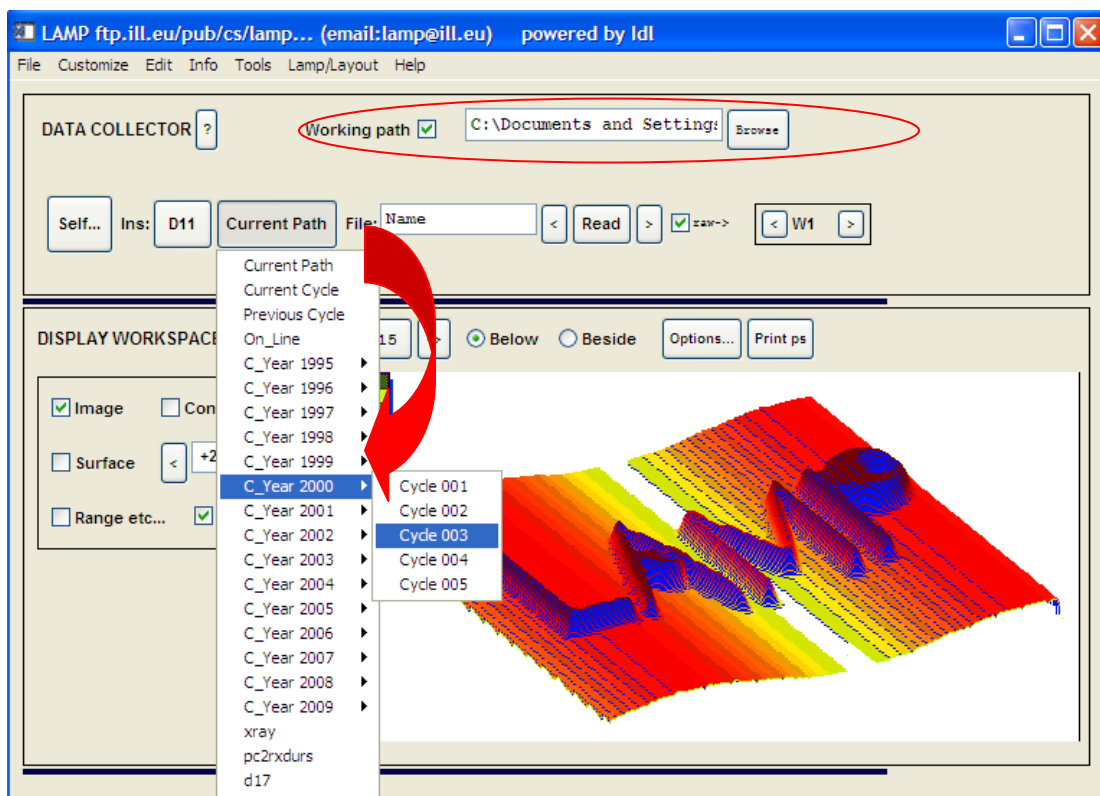
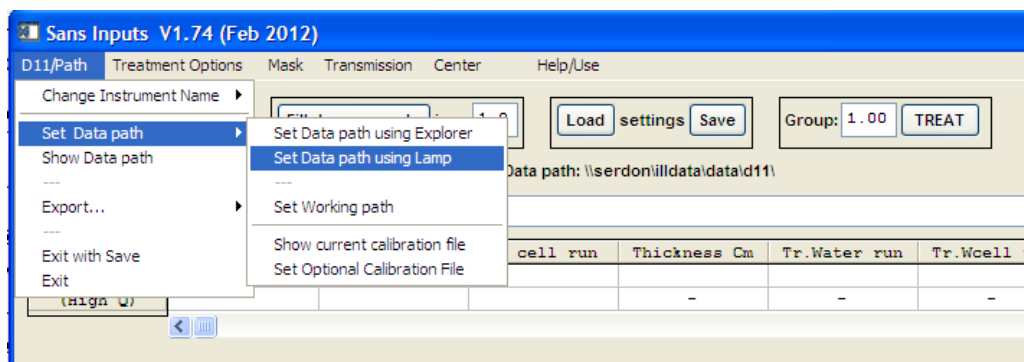


Figure 3.1: Setting the right path to look for the raw data. Inside the ILL they can be read directly from the data server (select year and cycle). Otherwise they need to be copied to the current working directory (check if the working path given in the text box is correct and browse the right one if not) and then the “Current Path” option has to be selected.

3) Fill the spreadsheet:

Now all the information concerning the experiment should be introduced in the table (Fig. 3.2). In a standard experiment this means that all the white cells will be filled. However in most cases the program will be able to deal with any missing information (i.e. cells not filled)¹. Light grey boxes are used to output the calculated transmissions. However if needed (e.g. a transmission has not been measured or the calculated value is incorrect) they can be edited and modified by the user. Finally the dark grey boxes are only used to provide some additional information concerning the numors read and they cannot be modified.

a. Water runs: The first block contains the series of measurements needed to calculate the detector efficiency map. In the first row the user should give the numors corresponding to a water run or any appropriate standard such as plexiglass or vanadium (typically measured with a detector distance between 4 and 10 m) and the corresponding background runs (Cd or B₄C and empty cell). The user also needs to provide the water thickness and the numors of the corresponding three transmission measurements (water, empty container and direct beam). The water signal is corrected and then employed to calculate the efficiency of each detector cell (see section on Data Treatment for more details). This efficiency map is then applied to all configurations (low, middle and high detector distances), unless a second water measurement is given.

There are some instrumental effects that cannot be corrected in a standard way, as they depend on specific instrumental details (see e.g [4-5]). Typically they result in a deviation from the assumed (for water) flat intensity at large Q values ($> 0.3 \text{ \AA}^{-1}$). To correct for this it is possible to provide a second water run measured at the same conditions as the “high-Q” sample. The “high-Q” water is then used to correct the “high-Q” runs, so all the geometrical and instrumental effects cancel. And the “default” water is employed to correct the “low-Q” and “middle-Q” runs. Note that in the case of D16 the sample to detector distance is fixed, so the terms low, middle and high-Q are replaced by scan 1, scan 2, and scan 3 (see section 7 for a more detailed discussion on how to treat D16 data).

A third possibility is that the user loads a calibration file (in the Treatment Options menu) containing the detector efficiency map. In this case the water measurement is not needed.

b. Direct beam and background runs: In the second block the user must provide the runs corresponding to the direct beam and the ancillary (electronic and container background) measurements. In the first row the numors corresponding to the direct beam²

¹ This includes missing background or absorbent measurements, as well as sample measurements. For example, we may have a series of samples measured at three different detector distances, while some others were only measured at two distances. The program will also be able to deal with the cases were the water run is missing (but then the correction by the detector efficiency cannot be performed, unless a calibration file has been previously loaded).

² This is a “transmission-like” measurements, i.e. with no beam-stop and an attenuator (if needed), and without any sample or container in the neutron beam. Hence the row name “Beam Tr.” They will be employed to determine the center corresponding to each configuration and to estimate the incident flux.

measured at the three distances corresponding to the “low-Q”, “middle-Q” and “high-Q” configuration should be given³. These runs are used to calculate the incident flux (using tabulated attenuator values) and to determine the beam center for each configuration. The number given in the 4th column of the 1st row is used to compute the transmission of the empty cell, so it must correspond to an acquisition taken with the same conditions as the rest of the transmission measurements (empty cell and sample). The second row will contain the electronic background measurements obtained with a Cd or B₄C sample. Finally in the third row the user must give the empty cell runs and the transmission measurement done with the empty container.

c. Sample runs: The third block is used to input all the sample measurements. The number of samples can be modified using the “Samples #” box (in the top line, below the menus). The “Cells...” and the “Fill down sample” buttons provide some utilities to modify the table and fill automatically the columns. The first column can be edited to give a sample name that will be used to identify the different samples in the results window (see below). The next three columns will contain the sample runs performed at one to three increasingly shorter distances corresponding to the “low-Q”, “middle-Q” and “high-Q” configurations. The following column is used to give the number of the transmission measurement for each sample. Finally the user must provide the sample thickness in the last white column to fill.

If a table has been completely filled the user can add further rows simply changing the number of samples in the corresponding box. If one prefers to add one row at the beginning or the middle of the table, then the option “Insert a new sample ID just before the selected one” in the “Cells...” button must be used. Note that this will add a row at the desired position, but it will not change the number of samples. Therefore if the table is full the user should change the number of samples before doing this or otherwise the sample in the last row will be lost. Finally the “Remove” option in the “Cells...” button allows deleting some rows.

Concerning the syntax to employ when more than one number needs to be read in one cell, there are different possibilities:

- 10 + 20 + 30 = Sums numbers 10, 20 and 30
- 10 > 15 = Sums numbers from 10 to 15
- 10 + 20>25 + 30 = Sums numbers 10, 20, 21, 22, 23, 24, 25 and 30
- 11:20 = Concatenates numbers from 11 to 20 creating a 3D workspace.
The 10 runs (numbers 11 to 20) will be treated as independent samples, but associated to the same transmission run (see section 6 on kinetic scans).
- 10, 15:20, 30 = Concatenates numbers 10, 15, 16, 17, 18, 19, 20 and 30 into a 3D workspace. As above they will be treated as independent samples, but sharing the same transmission run.

³ Naturally only the used configurations need to be filled.

Note that the numor concatenation can be employed either in the sample or in the cell background cells, as well as in the corresponding transmission runs. If several runs are concatenated in a sample cell and a single background run is given, this background will be applied to all the corresponding sample runs. If the same number of runs are concatenated in both a sample and the corresponding background cell then the program will associate a different background run to each of the sample runs. The same applies to the transmissions.

The data can be checked visually at any moment by “right-clicking” in any of the filled values. When doing this the raw data will be shown in another window (Fig. 3.3). Additionally, the main information concerning the selected numor will appear in the text line of the main window (see zone d in Fig. 3.2). Note that the number of counts given after the run title (read from the numor file) corresponds to the total counting in the detector excluding the default detector mask and any additional detector mask already defined and applicable to the displayed numor (e.g. if we have defined an additional detector mask for all angles the sum will not include the detector region corresponding to this mask, but if this additional detector mask has been defined only as a low angle mask it will affect the integration region only when displaying a low-Q measurement). If needed, the number of counts over the full detector (without masking any region) can be obtained by clearing all masks. This can be done by selecting one of the options under “Additional masks for detector” and then the option “Clear all masks” under the “Clear” button. The same button can be used to get back the instrument default mask.

Sans Inputs V1.74 (Feb 2012)

D11/Path Treatment Options Mask Transmission Center Help/Use

Cells... Samples # 3 Fill down sample incr: 0.0 Load settings Save Group: 1.00 TREAT

run 33418 Wavelength= 6.00 Distance:34.00 Collim:34.00 Offset: 0.00 Time(sec):2400 Count:AR PS3 0.4%,N=9909947

WATER RUNS. Notes->

	Water run	Cd/B4C run	W. cell run	Thickness Cm	Tr.Water run	Tr.Wcell run	Tr.Wbeam run
Default	33406	33408	33407	0.1	33397	33398	33399
(High Q)	33375	33377	33376	-	-	-	-

LOW ANGLE. Notes->
MIDDLE ANGLE. Notes->
HIGH ANGLE. Notes->

	LOW Q run	MIDDLE Q run	HIGH Q run	Transm. run	<-> Tr.value	-> Tr.error	-> Lo Counts
Beam Tr.	33423	33399	33384	33399	-	-	EB 34m,N=128954
Cd/B4C	33416	33408	33377	-	-	-	B4C,N=1018
Cell Bg.	33415	33407	33376	33398			EC 2mm,N=42427

SAMPLE inputs.

Sample IDs	LOW Q run	MIDDLE Q run	HIGH Q run	Transm. run	Thickness Cm	<-> Tr.value	-> Tr.error
AR PS3 0.4%	33418	33410	33379	33401	0.2		
AR PS3 0.1%	33419	33411	33380	33402	0.2		
AR PS3 0.025%	33420	33412	33381	33403	0.2		

Figure 3.2: Example of a filled table.

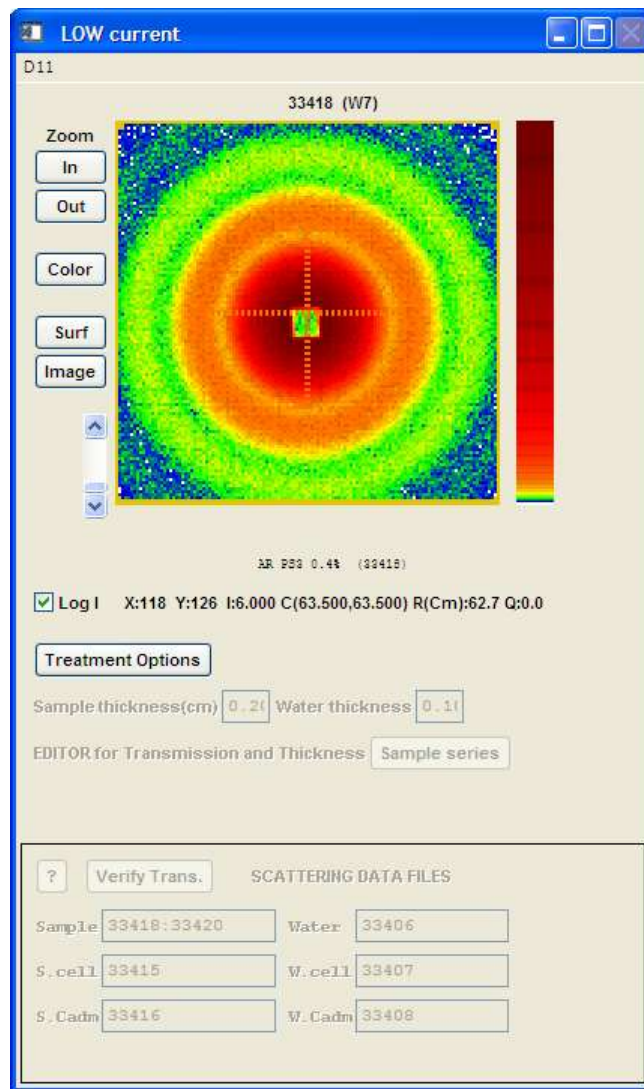


Figure 3.3: Window showing the raw data.

4) Check or modify the treatment options:

The first block in the “Treatment Options” menu contains a series of alternatives that can be activated or deactivated. They include the choices to calculate automatically the center, the transmissions and the masks, as well as the possibility to write automatically the final results and increment the file extension if a file with the same name already exists (this is valid only for the “G/T” files). The option “Re-read data input runs” can be activated to force the program to read again all the information from the numor data files instead of relying on the information already read and saved into memory. The **“Group Mode”** option allows selecting how to group the data⁴. The second block of options named

⁴ By default the program will do a radial integration, but it is also possible to do an azimuthal integration or to define a set of sectors and integrate over each of them.

“**Corrections**” will call the interface shown in Fig. 3.4, which allows selecting or changing the options to be used in the data correction procedure. Finally the last block contains two lines that allow loading a calibration file that will be applied to each of the numors read and showing the efficiency map currently in use. By moving the cursor on the window the user can check the values for the efficiency of each detector pixel, as well as the radial distance to the center of the pixel and the corresponding Q value.

Corrections applied: The window allowing selecting which corrections to apply in the data treatment (called from the line named Corrections in the Treatment Options menu) is shown in Fig. 3.4. The upper part of the window allows changing between the configurations by selecting Conf 1, 2 or 3 and provides a short summary of the conditions corresponding to the selected configuration: wavelength, detector distance, center, size of beam stop mask (if created), and collimation. A small 2D image of the data is shown and by clicking on it a larger image will appear. The user can move the mouse over the large image and the coordinates, intensity, distance to center and Q value of the current pixel will appear in the text line below the image. The buttons beside allow zooming in and out, as well as changing the color scheme or plotting a larger image as a 2D map or a surface. In order to return to the initial window the user can click on the “Treatment Options” button in the window. Finally the distance and collimation of the water measurement that is going to be used to calculate the efficiency map applied to the selected configuration are also shown.

The lower part of the window allows selecting the **corrections and options** to use in the data treatment: detector dead time correction⁵, solid angle correction⁶, normalization to monitor or counting time, and method to employ to obtain the absolute intensity (see section on data treatment and corrections).

Two other corrections that can be applied appear above (in the last line of the upper window) and allow correcting for the attenuation of the neutron beam scattered at an angle 2θ ($\text{Tr}(2\theta)$)⁷, and applying an instrument dependent correction⁸. By default all the

⁵ The number of counts is corrected in order to take into account losses due to the detector dead time. The right expression and detector dead time τ are automatically loaded for the instrument selected. The value of τ and the function to employ to correct for this effect can be modified manually, but this should only be done by the instrument responsible when the default values are no longer valid for a particular reason.

⁶ The solid angle of a detector cell of sides p_x and p_y is $\Delta\Omega(2\theta) = p_x p_y \cos^3(2\theta)/D$, where D is the sample to detector distance. As a consequence the measured intensity decreases proportionally to $\cos^3(2\theta)$. This effect is corrected by the solid angle correction.

⁷ This is done by introducing an angle dependent transmission, $T(2\theta)$, using the method suggested in [4].

⁸ There may be some small effects that are not fully accounted by the standard geometrical corrections (see e.g. [4-5]) and that typically cause deviations from the correct signal at large Q-values. An empirical function has been parameterized using a set of water measurements, in order to correct for the observed deviations from the expected flat signal. However it should be noted that the data set employed is still quite limited, so this correction may fail if the measurement has been done with a different configuration (wavelength, distance, and/or collimation). When two different water measurements are employed to calibrate the low/middle-Q and high-Q configurations, those instrument dependent effects will cancel, so the correction is not needed. In any case, the correction is applied to all the measurements, so even if the corresponding box is not deselected this will not have any influence in the result.

corrections are selected and should be applied, but in case of problems or doubts the user can decide which corrections to apply or not by deselecting the desired boxes.

The screenshot shows a software window titled "D11" with a blue border. The main area is titled "OPTIONS FOR DETECTOR CORRECTIONS". It contains several input fields and checkboxes. At the top, there are fields for "Wavelength (Å)" (5.999), "Distance (m)" (33.998), "Center (Px) CX" (63.500), "CY" (60.000), "Beam size X" (0.0), "(Px) Y" (0.0), "Offset (mm)" (0.000), and "Angle (deg)" (0.00). Below these are three radio buttons for "Conf 1", "2", and "3", with "Conf 1" selected. To the left of the radio buttons is a red square with a blue crosshair. To the right are fields for "Collimation (m)" (34.000), "Water Collimation" (8.0000), and "Water Distance" (7.9960). Below these are checkboxes for "Tr (2th)" (checked) and "Q dep" (checked). Further down are checkboxes for "Log I" (checked), "Dead Times" (checked), "Solid angles" (checked), and "Fixed Water Cross Section" (unchecked). The "Dead Times" section has a "Tau" field (4.20E-007) and a "Tau function" button. The "Solid angles" section has radio buttons for "use Monitor" (selected) and "use Time", and a "Group" field (1.0). The "Fixed Water Cross Section" section has a field (1.151), a "?" button, and a "No scaling" checkbox. At the bottom is a section titled "SCATTERING DATA FILES" with a "Verify Trans." button and fields for "Sample" (33418:33420), "Water" (33406), "S.cell" (33415), "W.cell" (33407), "S.Cadm" (33416), and "W.Cadm" (33408).

Figure 3.4: Interface to select/change the options to be used in the treatment.

Concerning the calculation of the absolute intensities, the default method employs the incident flux as estimated from the direct beam measurements performed at each detector distance in order to obtain the differential scattering cross-section per unit sample volume, $d\Sigma/d\Omega$ (cm^{-1}). However the precision in the estimation of the incident flux is limited [2], so a second possibility consists in using a standard sample (typically light water) of well known differential cross section and perform the scaling in relation to this sample. In this case the user should tick the box “Fixed Water Cross Section” and introduce in the

neighboring box the right value for the differential scattering cross section (in cm^{-1})⁹. Finally the user can tick the ‘No scaling’ option. In this case the data will be corrected, but no calibration will be performed. The help button provides some help about the formulas employed in each case. The equations applied and all the details concerning the data treatment are given in the ‘Data Treatment’ section.

5) Define the masks:

Use the “Mask” menu to define all the needed masks. The interface shown in Fig. 3.5 will appear and the user can use the left or middle mouse-button to select the area corresponding to the beam stop, such that this region will be masked. Once a region has been selected the corresponding values are shown in the box named ‘Beam x1, x2, y1, y2’. Those values can be edited and the masked region will change accordingly. The show button allows hiding or showing different masks, as well as changing the shape of the beam stop (rectangular or ellipsoidal). The detector image can also be zoomed (using the In button on the interface, Out to zoom out) and in this case the left mouse-button can be used to move the image and the middle button to define the mask.

The first three lines in the Mask menu allow defining the masks corresponding to the beam stop for the three detector distances. In each case only a single mask per configuration can be defined. When one of these lines is selected the lower part of the interface will show that the ‘Sample Beam’ option is selected and the number that is currently plotted in the figure. By default this is the empty cell measurement corresponding to the selected configuration, but the user can write a different number in the box and the window will show the desired data.

The following line allows defining the water mask. In this case the ‘Water Beam’ option will appear as selected in the lower part of the window, and the corresponding number appears in the Water box. Again only a single mask can be defined and in this case the values will appear in the “Box x1, x2, y1, y2” box. Note that the mask is defined for the currently selected water, so in case the user is using a second water for the high-Q configuration, he should create the mask for the default water, and then select the high-Q water and create another mask¹⁰.

The previous masks are employed only to cover the beam stop region. If the user needs to cover additional detector regions, he must use the menu ‘Additional masks for detector’. In this case he can create a mask for a particular configuration (e.g. to cover a parasitic reflection appearing at a particular sample-detector distance) or to be applied to all configurations (e.g. to cover a damaged detector region). Again the selected option (Cur Conf or All conf) will be shown in the lower part of the window, together with the plotted number. **If both a general mask and an additional mask for a given distance are**

⁹ The effective differential scattering cross-section of water depends on the wavelength and is instrument specific, so the needed value should be provided by the instrument responsible.

¹⁰ Note that if a water mask is not defined, but the program has a sample mask corresponding to an equivalent configuration (same distance and collimation), this mask will be automatically employed for the water. The same occurs if the sample mask is missing but there is a water mask available for this configuration. Finally if no masks are defined, the program will try to calculate them automatically, but it is not advised to rely on automatically calculated masks.

needed, the mask to be applied to all the detectors distances should be created first! The number of additional masks is unlimited, but only the coordinates of the last mask created appear in the “Box x1, x2,y1,y2” zone and can be edited. The “Undo” button removes only the last mask, but it can be applied consecutively to remove a given number of masks. The “Clear” button allows removing all detector masks, including the instrument default mask¹¹, or keeping only the default mask. Note that this button does not affect the beam stop mask.

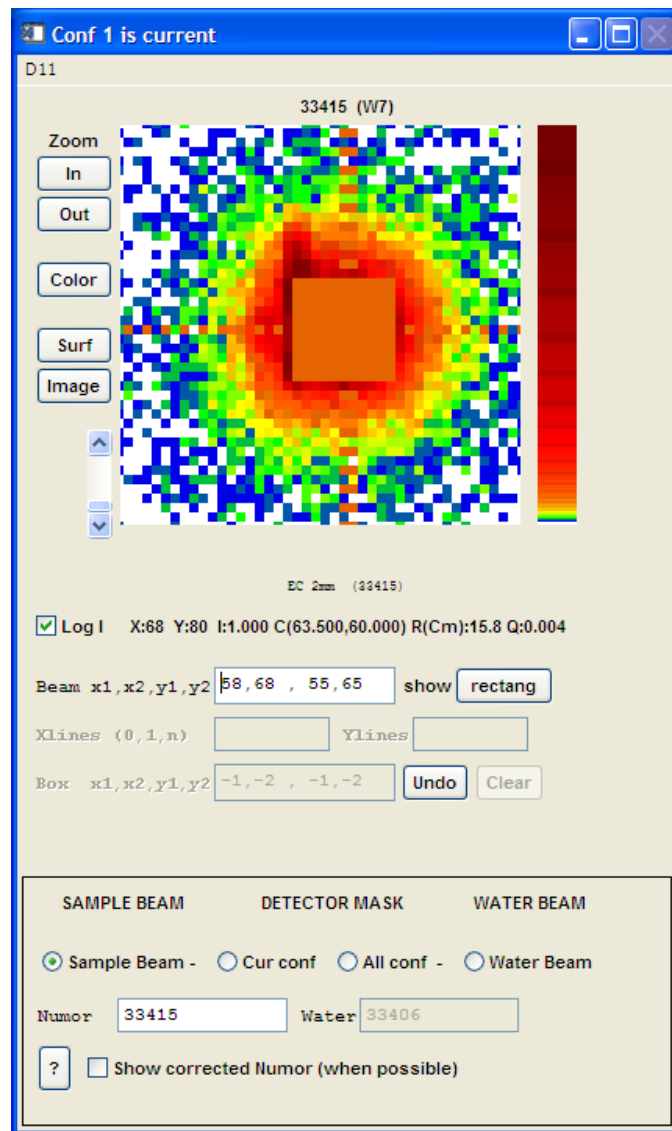


Figure 3.5: Interface to create a mask.

6) Calculate the transmissions:

¹¹ The instrument default mask is defined for each instrument (typically it covers one or several of the most external detector lines) and it is always applied by default.

The transmissions can be automatically calculated by the program (see option in menu “Treatment Options”) and in most cases the result is very reliable¹². However the user can check the calculation using the menu “Transmissions”, that will make appear a window like the one shown in Fig. 3.6. When this window appears the total number of counts inside the integration region for the direct beam is given. If no region has been selected, the number given corresponds to the sum over the full detector but excluding the region masked by default. If the user wants to know the total number of counts in a particular region, he/she can sketch the integration region and then replot the window by calling it from the Transmissions menu and the number of counts will be updated.

The user can then define the desired integration region using the mouse left-button (middle-button if zoomed image) and then click on “Calculate Transmission” to perform the calculation. The calculated transmissions will then be filled directly into the main table. Note that the transmission values of the main table can be edited, so if for any reason the user prefers to change any of the calculated values he can do it and the modified transmissions will be used in the data treatment. The computed transmissions are also saved in an ASCII file named *sans_transmissions.txt* and they can be reloaded if needed using the option “Get transmissions from an input file”.

7) Calculate the center for each configuration:

As for the transmissions, the center can be automatically calculated (option in Treatment Options), although it is a good practice to check the result. The “Center” menu allows calculating the center for each of the configurations employed. A window similar to the one shown in Fig. 3.7 will appear, allowing the user to define a given range to calculate it. Then the beam center is computed as the center of gravity of the neutron counts inside the selected region. However the user can also choose to determine the beam center from a fit to a double Gaussian function or as the average between both methods. In standard situations, the result will not change, but there may be particular cases where one option could be preferred (e.g. if the beam center is shifted almost outside of the detector). The calculated center (CX, CY) is shown in the center interface and written in the comments block of the main table as well. The estimated incident flux for the present configuration (Φ_0) is also shown in the interface.

The user can fix a specific center by giving a single value in the Xrange and Yrange boxes (see Fig. 3.7). This can be useful for comparison purposes or when a valid direct beam measurement is not available to determine the center.

A final remark is that at the same time that the calculation of the center is done, the width of the neutron beam is also computed from a double fit to the horizontal and vertical

¹² The automatic transmission calculation is simply done using the ratio between the total number of counts corresponding to two direct beam measurements (sample/water and empty cell or empty cell and empty instrument). So as long as the total number of counts is really representative of the transmitted intensity, the calculated transmissions will be correct. Errors could appear only in particular situations if a significant part of the total detected neutrons do not come from the transmitted beam, e.g. if there is a problem with a detector pixel having a very large electronic background or we have a very large (compared to the transmitted beam) scattering signal from the sample entering into the detector.

profiles. This value is used to compute $\sigma(\Theta)$ which is later employed to calculate the Q-resolution (see section 4.9). As the fit is done only over the region selected to compute the center, the width obtained may be largely overestimated if the number of pixels selected is too small. Therefore the user is recommended to use the full detector when computing the beam center or at least a reasonable detector window extending well into the region where the number of counts is close to zero (typically a window of 20 x 20 pixels is enough to avoid any problems with the automatic fitting procedure). This also implies that when the center is set manually the value of $\sigma(\Theta)$ is not known and the Q-resolution cannot be computed.

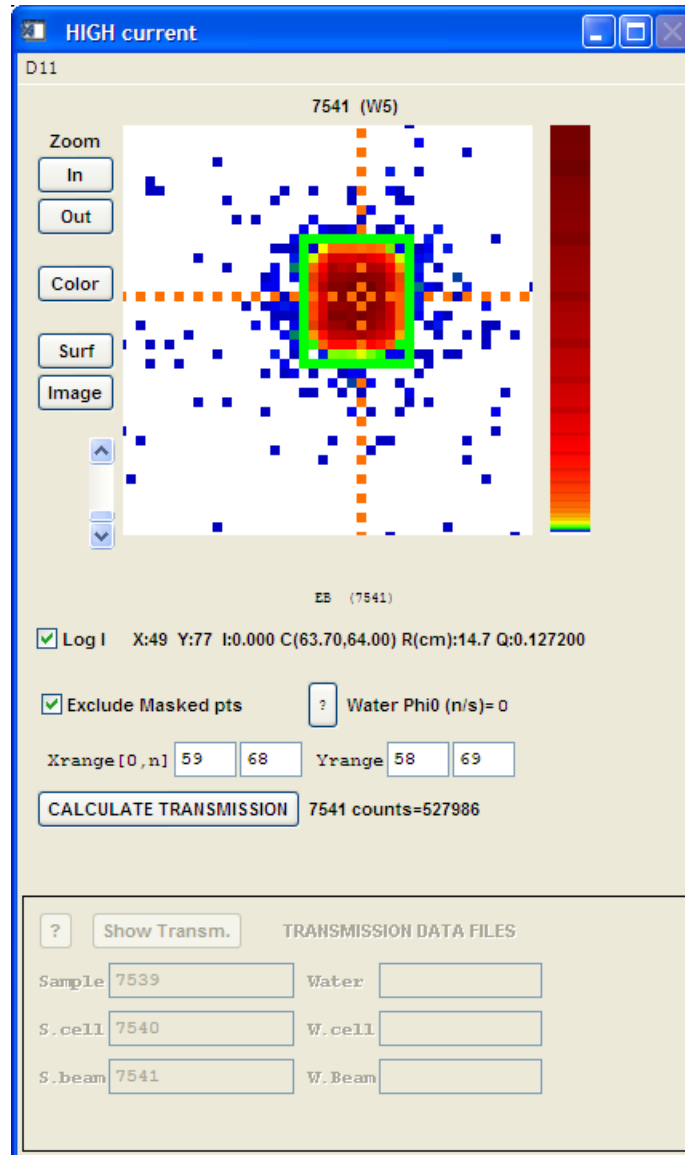


Figure 3.6: Interface to calculate the transmissions.

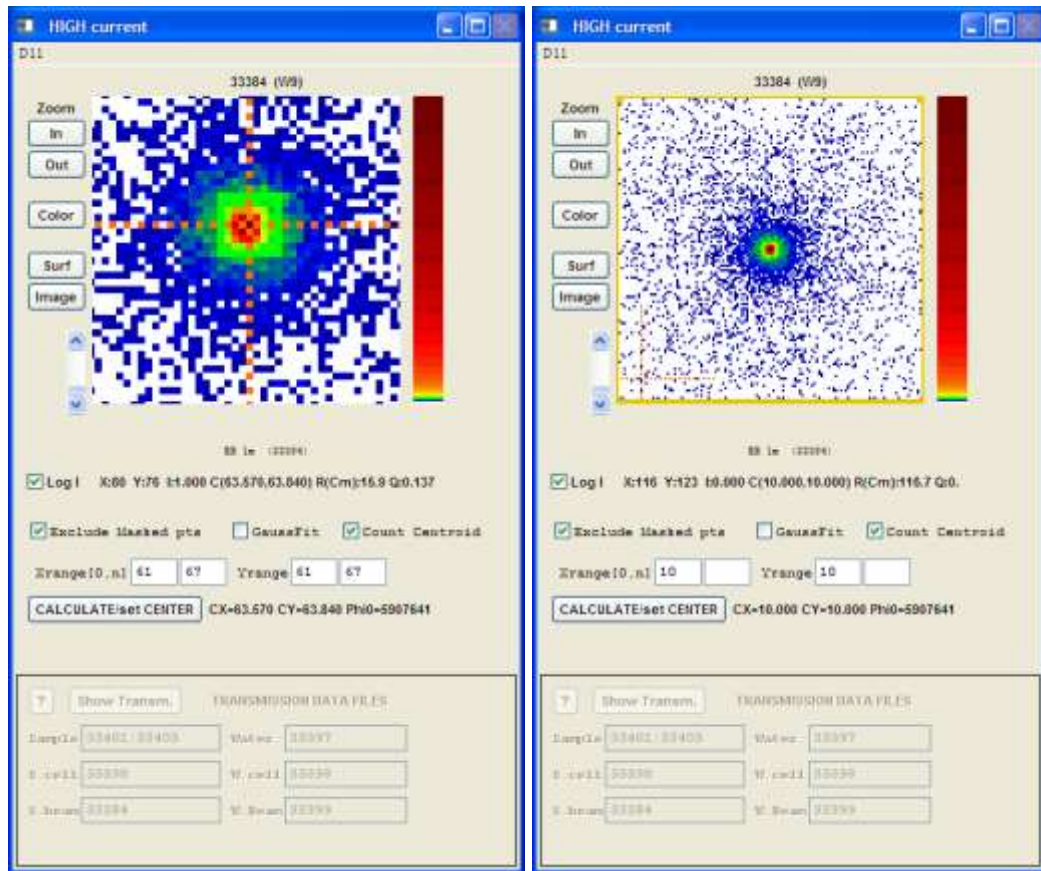


Figure 3.7: Interface to calculate the center. The right figure shows how to specify the center at a particular position (in this case at the pixel (10, 10)).

8) Treat:

Now the data reduction can be done using one of the different possibilities that appear under the “Treat” button (see Fig. 3.8). The “Group” box beside this button allows to choose the step (in pixels) to be employed when integrating the data. The standard value to use is 1.0, while setting the value to 0.0 means that the data will be corrected but not integrated, resulting in a series of 2D files¹³. The user can choose to treat all the configurations at the same time or just a particular one. Once the treatment is completed, a window to plot and manipulate the results will appear (Fig. 3.10). At the same time, the dark grey cells (Lo counts, Md counts, Hi counts) of the spreadsheet will be filled with the numor title and the total number of counts, so this can be used to check that all the input numors were correct. Note that the number of counts is the sum over the full detector excluding any detector mask (see comments on section 3.3). Note as well that if the table is already filled and a second treatment with different detector masks is performed, the values in those cells will be updated only if the option “Re-read data input

¹³ Note that even when the data are integrated, the 2D corrected files are conserved and can be visualized and saved.

runs” has been selected in the “Treatment options” menu. Every time that a treatment is performed an ASCII file named *current_spreadsheet.txt* is written. This file contains all the information filled in the spreadsheet and therefore can be associated to the results to know exactly which operations have been performed to arrive to those results. Some basic information (particularly useful when something goes wrong) is also written in the Lamp Journal. This is accessible from the “Help/Use” menu, under the line “The JOURNAL” and its appearance is shown in Fig. 3.9. The method employed to obtain the absolute intensities is written (e.g. Efficiency scaling with $\phi = \dots$ or Water scaling with $F_{sc} = \dots$, $\chi_{H_2O} = \dots$, see 4.8 for more details) together with the distances and collimations corresponding to each configuration, so the user can check quickly if there is any problem with any of those basic parameters (e.g. due to a bad input in the table).

Another useful feature in the “Help/Use” menu is provided by the “Data inspection in LAMP” tool. SANS spreadsheet is linked to Lamp and uses the Lamp workspaces. This line shows the content of each of the workspaces employed by SANS spreadsheet, so it is possible to use the full functionality of Lamp for data inspection.

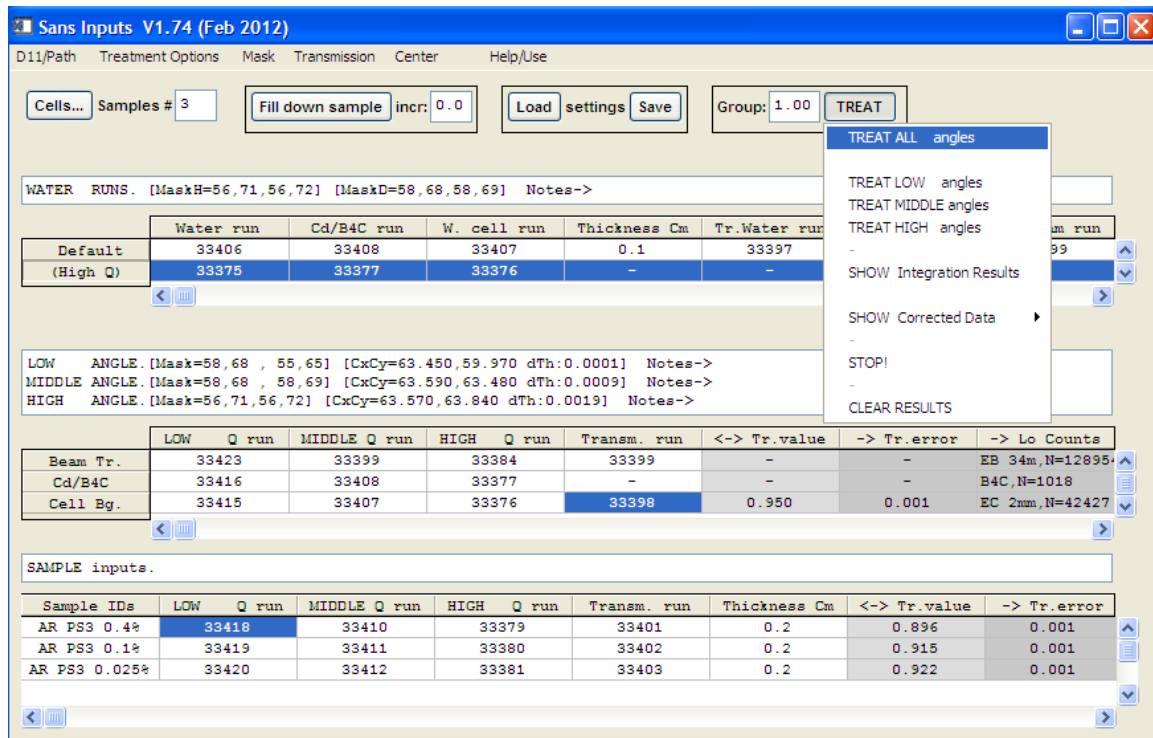


Figure 3.8: Launching the data reduction procedure.

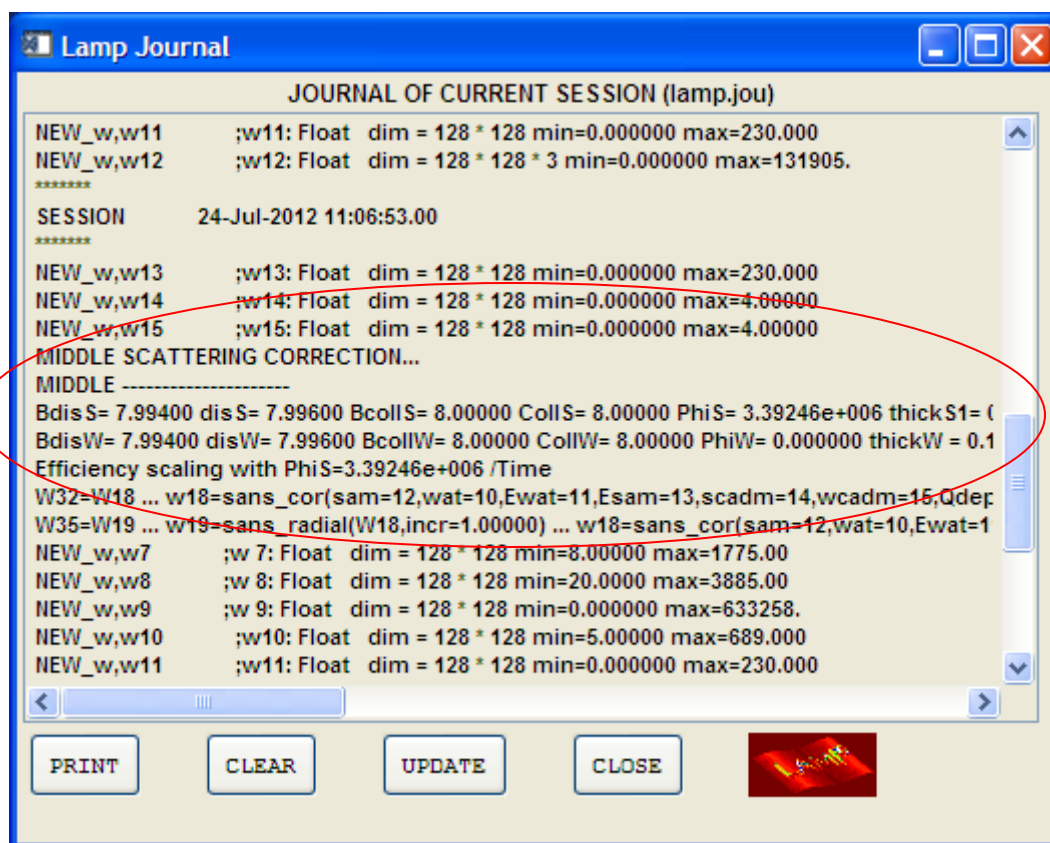


Figure 3.9: Lamp Journal. The conditions employed to reduce the middle-Q configuration (distances and collimations for sample, empty beam and water runs, as well as measuring times and monitor values) are shown.

9) Looking and manipulating the results:

Once the data treatment is done, the list of reduced data appears in the lower box of the interface shown in Fig. 3.10. This window can also be called from the “Treat” button, selecting the line “Show integration results”. It is also possible to plot the 2D corrected data by choosing “Show corrected data” and then “Show corrected LOW, MIDDLE or HIGH”.

In the text box of the results window shown in Fig. 3.10 each line corresponds to one particular sample and configuration and provides some information to identify the corresponding measurement (numor, configuration keyword: gH for High-Q, mM for Middle-Q, pL for Low-Q, title, wavelength, detector distance, collimation, etc.). The user can select one or several results and plot them in the graphical window. The type of scale and representation can be modified using the “Log I” button and the different possibilities available from the f(I) and f(Q) buttons, while the intensity and Q-ranges can be set manually by selecting “I rg” and/or “Q rg” and using the corresponding boxes to provide the desired limits. The list of data can be reordered using the button “Sorting and Selecting the List”, which allows as well selecting all the curves or all the samples measured at a given distance (Conf 1, 2 or 3 curves).

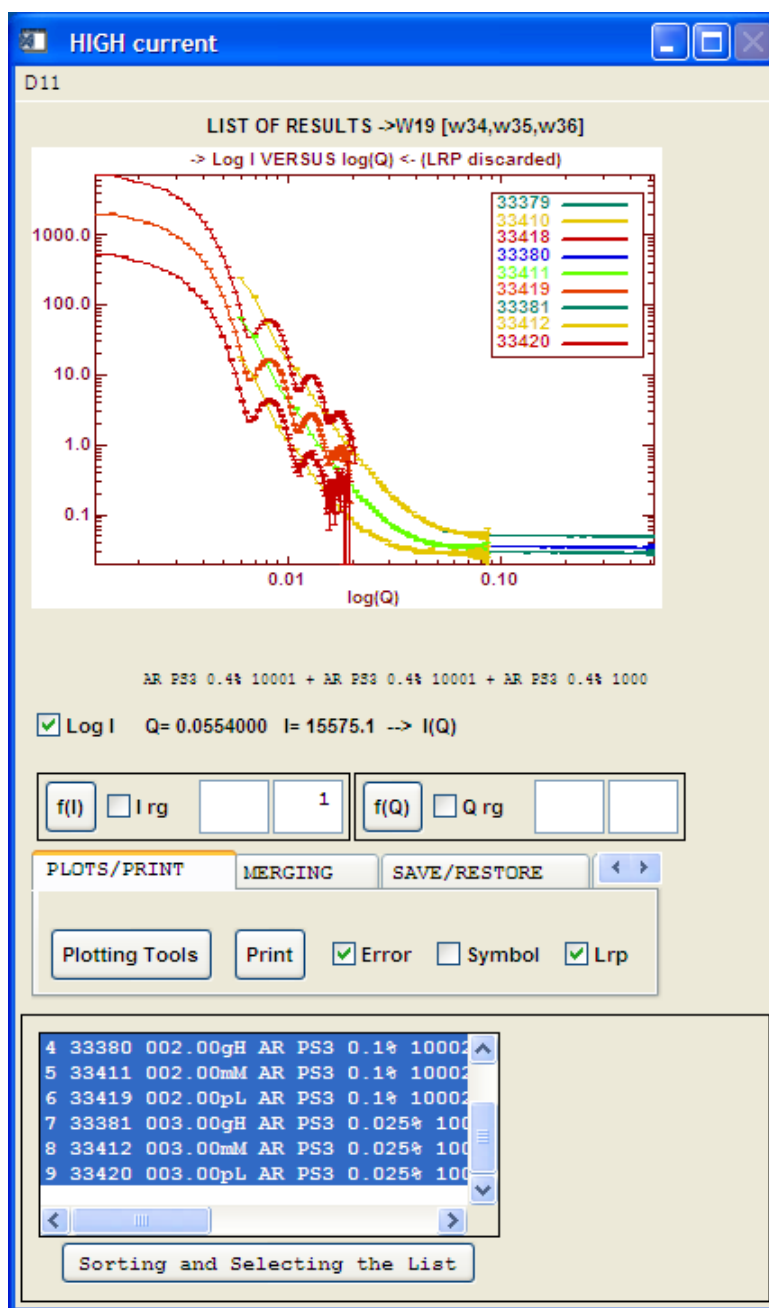


Figure 3.10: Interface to plot and manipulate the corrected data.

The results interface provides different options to display and manipulate the reduced curves. They are accessible from the tabs Plots/Print, Merging, Save/Restore, Operations and Models. The first one (“PLOTS/PRINT”) allows selecting the line style (lines or symbols, error bars or not), as well as printing the displayed image (to a postscript file or to the default printer). The “Lrp” box can be selected to discard “bad” points¹⁴. The

¹⁴ At present points are considered “bad” if their intensity is smaller than 10^{-7} or their error bar is 4 times larger than the intensity (only if $I_{\text{point}} > 1$).

“Plotting tools” provides different options to send the current figure to the Superplot tool available in Lamp or to the IDL iTools utility (by selecting Annotation Tool), where further options to edit the figure are available (see Fig. 3.11). There are also two additional options to create 2D or surface plots which are particularly adapted to display a series of kinetic runs, in order to observe the evolution in time of the scattering signal.

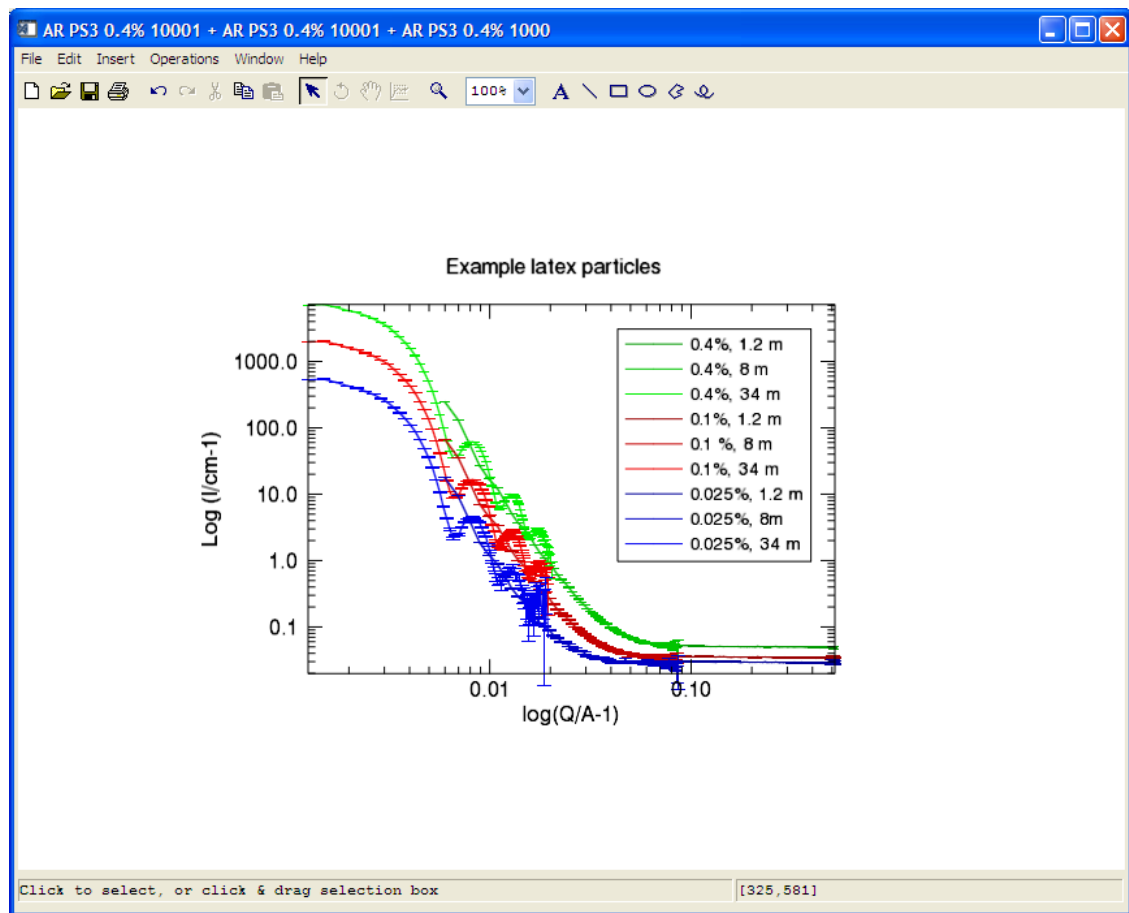


Figure 3.11: iTools interface.

The “MERGING” menu provides different possibilities to remove points, scale the curves or merge them. They can be accessed from the “Action” button (see Fig. 3.12). The “Qrange” input gives the possibility of selecting a particular wavevector range for each of the configurations (l: Low-Q, m: Middle-Q, h: High-Q), so this option can be employed to remove some points from each of the three curves (e.g. to eliminate points with large error bars or low Q resolution). Fig. 3.13 shows an example where overlapping points from different detector distances have been removed.

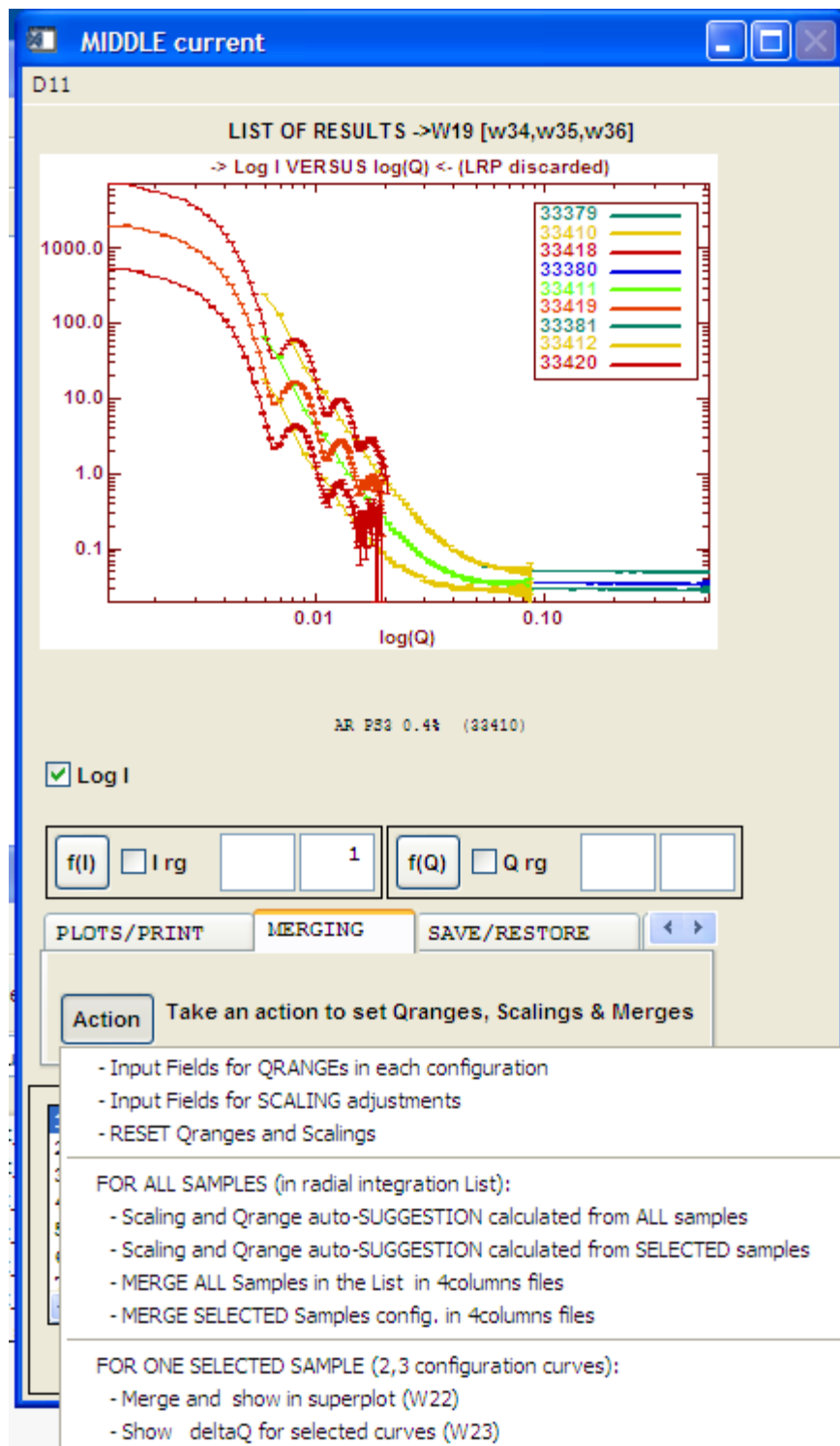


Figure 3.12: Merging options.

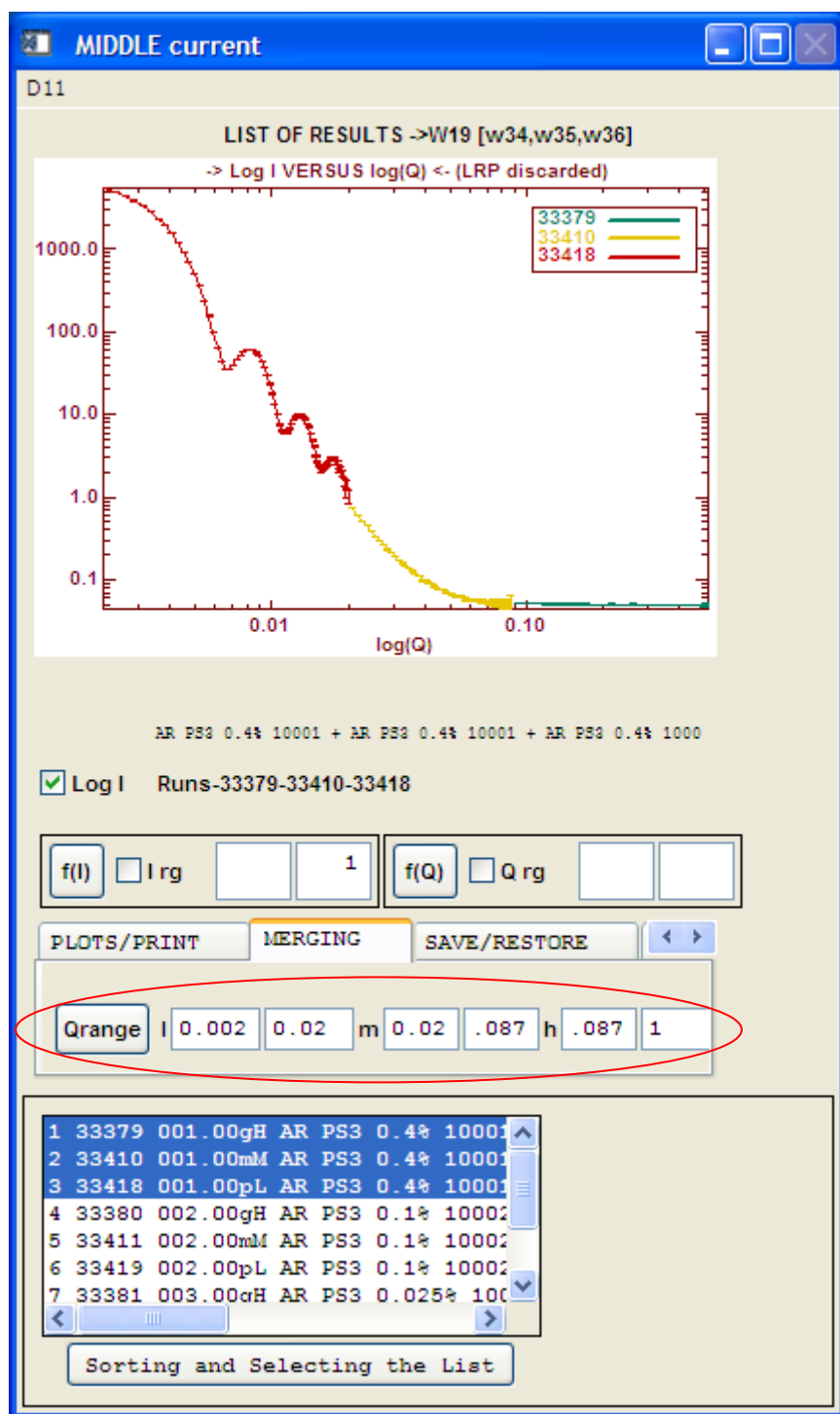


Figure 3.13: Removing overlapping points.

The “Scaling” lines allow applying a multiplication factor to the full set of curves corresponding to a particular detector distance (low, middle, high). This can be useful when one set of curves has not the correct intensity (e.g. if a good empty beam measurement is not available), so this “ad hoc” factor can be employed to rescale these curves to the same absolute intensity than the other sets. The Q-ranges and the scaling factors can be estimated automatically by the program using the full set of results (auto-suggestion from all samples) or just some selected curves (auto-suggestion from selected samples). The factors employed will be shown in the corresponding boxes (see Fig. 3.14).

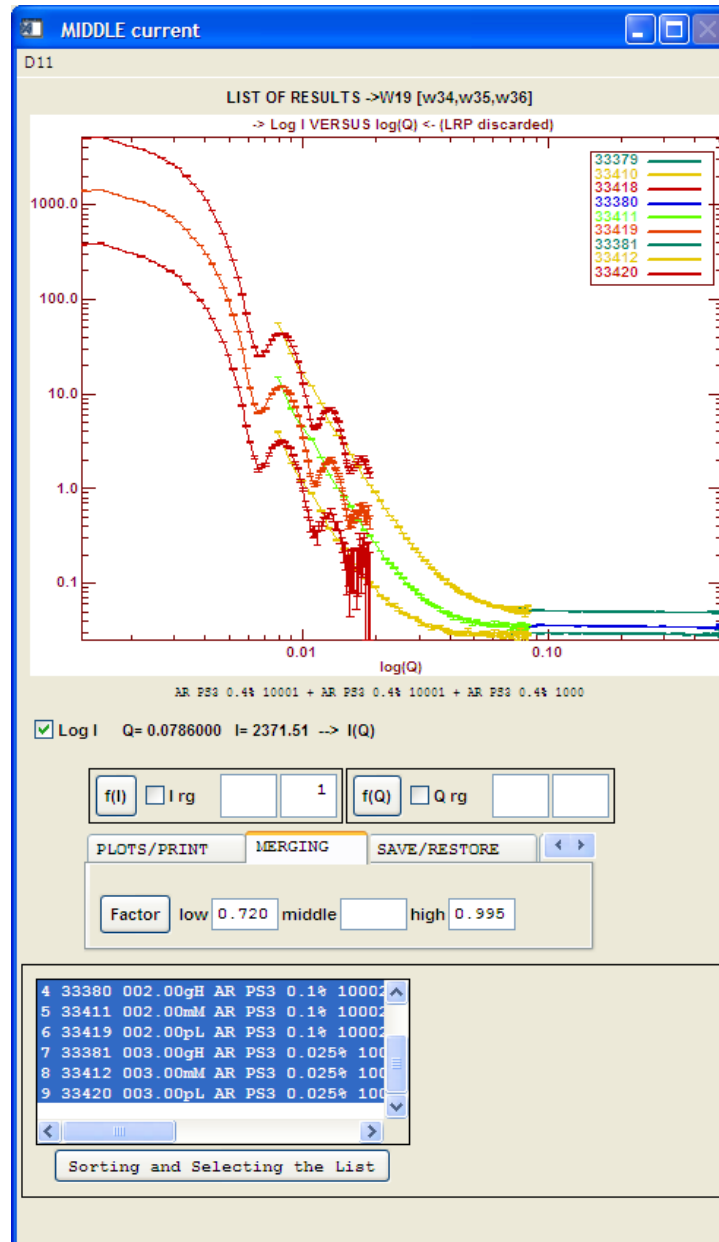


Figure 3.14: Auto-scaling option.

The following two lines in Fig. 3.12 (Merge ... and Show delta Q ...) allow merging automatically all or the selected samples into a single curve that will be exported as an ASCII file into the working path. The automatic merging is done by removing the bad points and then choosing the points with the best Q-resolution in the range where two configurations overlap. The export files are named "Instrument + _merge_ + numers + .txt" and contain 4 columns corresponding to Q, intensity, error in intensity and Q-resolution (σ). Finally the user can select only the 2 or 3 curves corresponding to a single sample and plot them or the corresponding resolution as a function of Q using Superplot.

The list of results can be saved and restored at a later time using the "SAVE/RESTORE" menu. The merge option available in the "Save/Restore LIST" button allows adding the new results to an existing list. If an old list is not available, but the data were exported into the "G(hosh)" format, they can be added to the present list using the button "Get gnum.* files". If a list exists and a new treatment is done, the new data will be added to the list, while "re-treated" data will be overwritten. It is also possible to clear completely the list of results before doing a new treatment by using the 'Clear List' button.

The menu "OPERATIONS" can be used to perform simple additions and subtractions between sets of data. The user can select one or several curves in the list of results and click on "Select 1", and then repeat the operation and click on "Select 2". The operation to be performed is shown schematically below the graphics window (e.g. [9,10,11,12] – [7]*0.1) and will be done when pressing the "Do" button. The resulting curves are added to the list of results.

Finally the menu "MODELS" provides some fitting utilities and a small library of standard models that can be employed to perform some preliminary analysis of the results.

10) Save the table and the results:

The table can be saved using the available button in the main interface (Fig. 3.15). This will save a binary file (.sav) containing all the information needed (including the full data) to redo the treatment. When a table is saved after the treatment has been done, the corresponding list of results is also saved (the name of the file will be the same as for the table, but adding the extension _result). Therefore it is possible to reload at a later time the table file in order to redo the treatment after modifying some options or adding some samples, or to simply load the file containing the list of results in order to plot or work on them. When saving a table, a text file (.txt) is also created. It is equivalent to the file named "current_spreadsheet.txt" that is written each time that the "Treat" button is pressed and contains a summary of the main information given in the table in a format that can be easily printed.

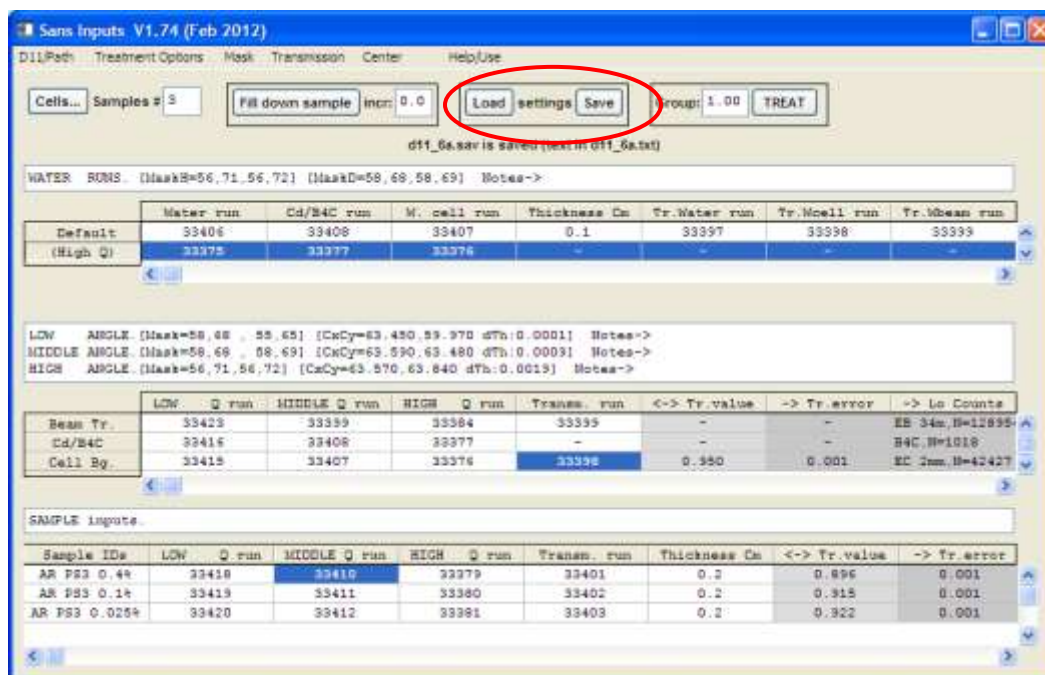


Figure 3.15: Saving and loading a filled table.

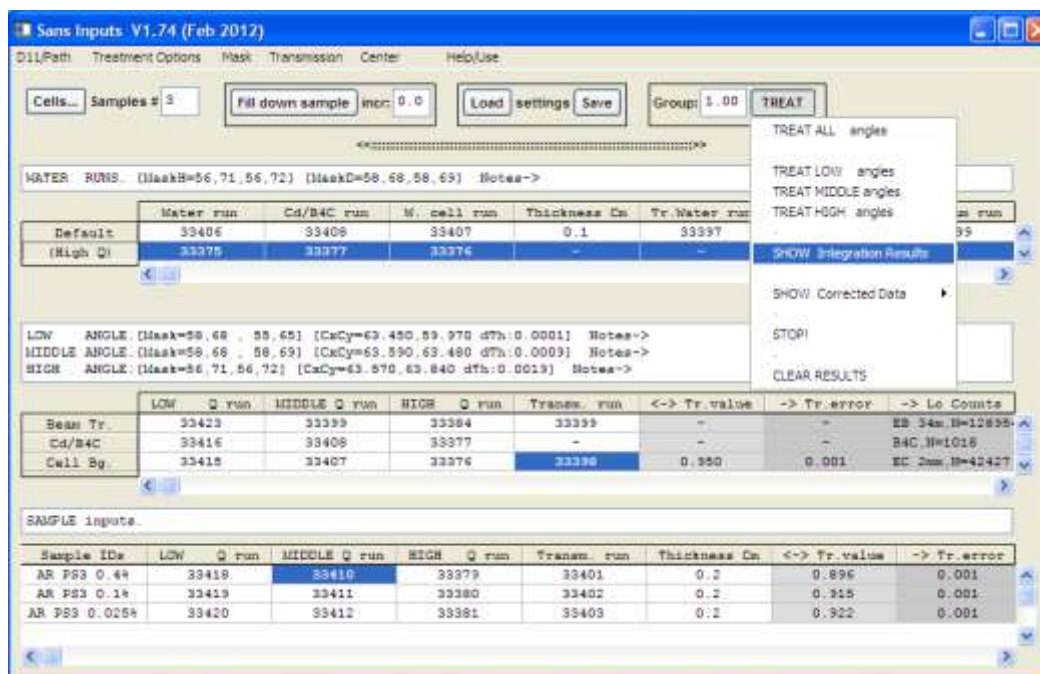


Figure 3.16: Showing the list of results.

Finally the integrated 1D curves or the corrected 2D data can be saved employing the “Export ...” button under the Instrument menu (Fig. 3.17). All the results are saved automatically using standard default names depending on the option chosen:

a. gnum.100: The name of the file will be gNNNNNN.EEE, where NNNNNN corresponds to the numor number and EEE is an extension number (100 by default and then increasing numbers if the treatment is repeated and the “Auto_increment resulting FILES” option in the menu “Treatment Options” is ON). In this case the data are saved in a format similar to that employed in the SANS data treatment suite of Ron Ghosh [1], so they can still be read and manipulated with the programs of that suite.

b. tnum.100: As above, but for 2D (not integrated) corrected data. Additionally the Q-value corresponding to each detector pixel is written into a different file for each of the configurations.

c. 1D_numor.txt: The name of the file will be INST_1D_NNN_INDEX.txt, where INST is the instrument name, NNN is the numor, and INDEX corresponds to the sample number in the table (starting from 0). In this case the data are saved as a simple ASCII file containing some comment lines followed by 4 columns giving Q (\AA^{-1}), I(Q), ΔI , and $\sigma(Q)$.

d. 2D_numor.txt: As above, but the name will be INST_2D_NNN_INDEX.txt and the detector image will be saved as an ASCII file containing N_x+1 columns and N_y+1 rows, where N_x and N_y are the detector dimensions. The first row of the file is a comment and the second contains the horizontal pixel number, while the first column gives the vertical pixel number. As in b), the Q-values of each detector pixel are also exported.

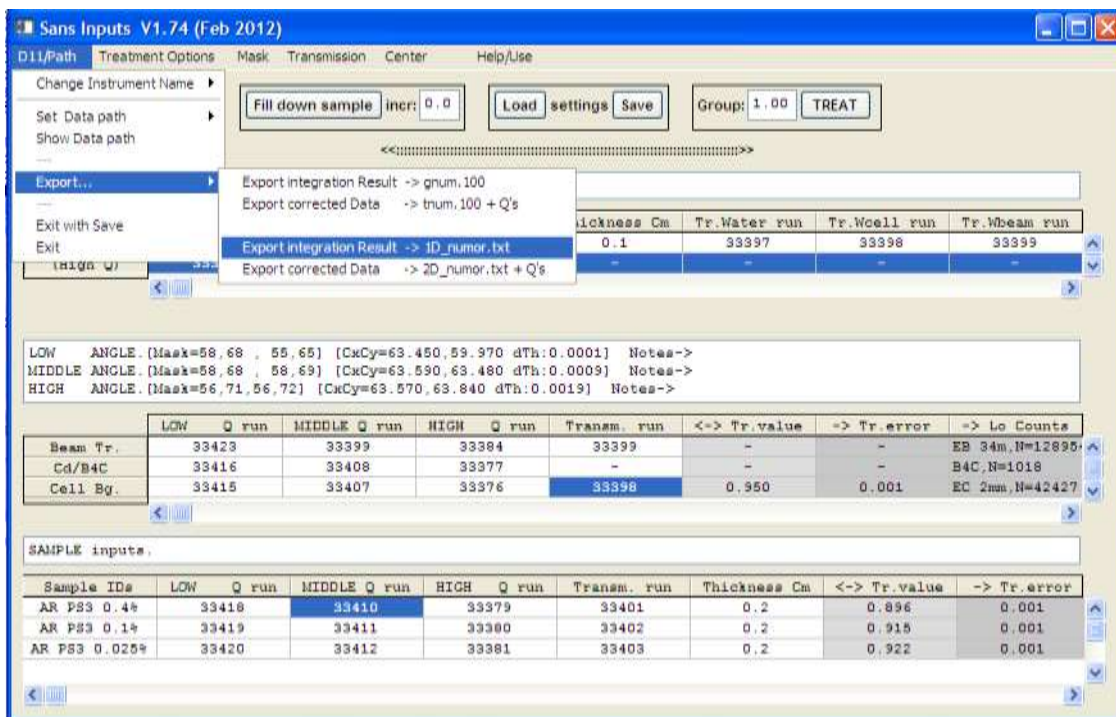


Figure 3.17: Exporting the data.

4. Data treatment and corrections applied

When clicking TREAT the program will perform the data reduction and will open a window containing the results for each sample and configuration measured. When the standard data treatment is performed, the output given corresponds to the absolute differential scattering cross section, calculated as:

$$\left(\frac{d\Sigma}{d\Omega}\right)(2\theta) = \frac{\left[\frac{I_s(2\theta) - I_{cd}(2\theta)}{T_s(2\theta)T_{ec}(2\theta)} - \frac{I_{ec}(2\theta) - I_{cd}(2\theta)}{T_{ec}(2\theta)}\right]}{t_s \cdot \Delta\Omega(2\theta) \cdot \varepsilon_{xy} \cdot \text{time} \cdot \Phi_0} (\text{cm}^{-1}) \quad [\text{Eqn. 4.1}],$$

where I_s , I_{ec} , and I_{cd} are the measured signals from the sample, the empty container and the absorbent (Cd or B₄C), respectively. The measured counts are corrected for the effect of the detector dead time, unless the option “*Dead Times*” is untoggled (see “Treatment Options: Corrections”). $T_s(2\theta)$ and $T_{ec}(2\theta)$ are the transmissions of the sample and the empty container, respectively, both of them corrected for the attenuation of the neutron beam scattered at an angle 2θ (see below). The reference transmissions are:

$$T_s(0) = \frac{I_s(2\theta=0)}{I_{ec}(2\theta=0)} \quad [\text{Eqn. 4.2}],$$

$$T_{ec}(0) = \frac{I_{ec}(2\theta=0)}{I_{db}(2\theta=0)} \quad [\text{Eqn. 4.3}],$$

where $I_{db}(2\theta=0)$ is the measured intensity for the direct beam without any sample or container at the sample position. In the first equation t_s is the sample thickness, $\Delta\Omega(2\theta)$ the solid angle covered by the pixel corresponding to the angle 2θ , ε_{xy} is the efficiency of each pixel in the detector, as determined from the water measurement, time is the counting time in seconds, and Φ_0 is the incident flux estimated from a direct beam measurement performed under the same configuration that the sample measurement.

The full correction treatment is done by the *sans_cor* procedure, where the following steps are performed:

1. The necessary parameters for a given configuration (Low Q / Middle Q / High Q) are read. This includes information such as the sample to detector distance and counting time, but also the position of the beam center for this particular configuration and all the transmissions calculated previously.
2. The beam center is used to compute the angle 2θ corresponding to each detector pixel.
3. All the measured counts are corrected for the effect of the detector dead time. At present (1st June 2012) the corrections applied by default are:

$$I_{xy}^{corr} = I_{xy} / \left[1 - \left(\sum_{xy} I_{xy} \right) \cdot (\tau/t) \right] \quad [\text{Eqn. 4.4}],$$

for D11, with $\tau = 4.2 \times 10^{-7}$ s, and

$$I_{tube}^{corr} = I_{tube} / \left[1 - \left(\sum_{tube} I_{tube} \right) \cdot (\tau/t) \right] \quad [\text{Eqn. 4.5}]$$

for D22, where the correction is applied tube by tube with $\tau = 2.0 \times 10^{-6}$ s.

If needed, the dead time correction can be deactivated by untoggling the “Dead Times” checkbox.

4. The attenuation of the neutron beam scattered at the angle 2θ with respect to the transmission measurement performed at $2\theta=0^\circ$ is taken into account by using an angle dependent transmission calculated using the approximation given by Brûlet et al. [4], i.e.:

$$T(2\theta) = T(0) \cdot \varepsilon_1[\alpha(2\theta) \cdot \ln T(0)] \quad [\text{Eqn. 4.6}],$$

with

$$\varepsilon_1(x) = 1 + x/2 + x^2/6 + x^3/24 + x^4/120 \quad [\text{Eqn. 4.7}],$$

$$\alpha(2\theta) = (1/\cos 2\theta) - 1 \quad [\text{Eqn. 4.8}].$$

As for the dead times, the angle dependence of the transmissions can be disabled using the corresponding checkbox, Tr(2th). In this case, a constant transmission $T(2\theta=0^\circ)$ will be used in the correction procedure.

5. The efficiency of each detector pixel is evaluated from the water measurement, once the latter is correctly treated. The correction includes the subtraction of the water container:

$$I'_w(2\theta) = I_w(2\theta)/T_w(2\theta) - I_{\text{ew}}(2\theta) \cdot (N_w/N_{\text{ew}}) \quad [\text{Eqn. 4.9}],$$

followed by the subtraction of the absorbent measurement:

$$I''_w(2\theta) = I'_w(2\theta) - (1/T_w(2\theta) - 1) \cdot I_{cd}(2\theta) \cdot (N_w/N_{cd}) \quad [\text{Eqn. 4.10}].$$

And this result is finally divided by the transmission of the empty cell and the solid angle factor, $\cos^3(2\theta)$, so we have:

$$I'''_w(2\theta) = I''_w(2\theta) / [T_{\text{ew}}(2\theta) \cdot \cos^3(2\theta)] \quad [\text{Eqn. 4.11}].$$

Here I_w , I_{ew} , and I_{Cd} are the measurements corresponding to the water sample, empty container used for the water, and absorbent, respectively. N_w , N_{ew} , and N_{Cd} are the corresponding monitor (or counting times if the corresponding option is selected) values for each acquisition. They are only used to normalize the background and absorbent measurements with respect to the water one. The combination of the previous three equations leads to:

$$I_w'''(2\theta) = \left[\frac{I_w(2\theta) - I_{Cd}(2\theta)}{T_w(2\theta)T_{ew}(2\theta)} - \frac{I_{ew}(2\theta) - I_{Cd}(2\theta)}{T_{ew}(2\theta)} \right] \cdot \frac{1}{\cos^3(2\theta)} \quad [\text{Eqn. 4.12}].$$

Then a reference value I_{ref} is defined as the median of all the values of $I_w'''(2\theta)$ after excluding the region defined with the water mask. And the efficiency of each pixel is simply calculated as $\epsilon_{xy} = I_w'''(2\theta)/I_{ref}$.

Note that the solid angle factor accounts for the different solid angle covered by each of the detector pixels, so normally should always be applied. However for testing purposes can be also deactivated using the “Solid angles” checkbox in the window of the Corrections menu.

In the case that two water measurements obtained at two different detector distances are given, two different efficiency maps will be calculated and applied, one to the low and middle configurations and another to the high-Q one. In this way the different distance-dependent geometrical corrections cancel for the middle and high-Q configurations when the sample and water measurements have been obtained using exactly the same conditions¹⁵.

6. The sample data are corrected in a similar way. First the signal from the sample container is subtracted:

$$I_s'(2\theta) = I_s(2\theta)/T_s(2\theta) - I_{es}(2\theta) \cdot (N_s/N_{es}) \quad [\text{Eqn. 4.13}].$$

Then the absorbent measurement is subtracted:

$$I_s''(2\theta) = I_s'(2\theta) - (1/T_s(2\theta) - 1) \cdot I_{Cd}(2\theta) \cdot (N_s/N_{Cd}) \quad [\text{Eqn. 4.14}].$$

And finally the result is divided by the transmission of the empty container and by the solid angle factor giving:

$$I_s'''(2\theta) = \left[\frac{I_s(2\theta) - I_{Cd}(2\theta)}{T_s(2\theta)T_{es}(2\theta)} - \frac{I_{es}(2\theta) - I_{Cd}(2\theta)}{T_{es}(2\theta)} \right] \cdot \frac{1}{\cos^3(2\theta)} \quad [\text{Eqn. 4.15}].$$

¹⁵ This procedure relies on the assumption that the water run provides an accurate measurement of the efficiency of the detector, i.e. that the intensity scattered by the water sample is uniformly distributed over the full solid angle covered by the detector.

7. An additional instrument dependent correction can be applied in order to correct for specific effects such as the parallax of the D22 detector or the deformation of the D11 membrane. This correction can be switched on and off using the “Qdep” toggle button. This part is still subject to future developments, but the functions currently tested and proposed for D11 and D22 are discussed in the appendixes 1 and 2.

8. The final result returned by the correction procedure depends on the option selected in the Corrections window called from the “Treatment Options” menu. There are several possibilities:

A. In the default case, the differential cross section of the sample is computed in absolute units using the estimated neutron flux. The latter is calculated from the direct beam measurement as $\Phi_0 = \frac{I_{tot}}{t} \cdot F_{att} \text{ (n/s)}$, where I_{tot} is the total number of counts detected corrected by the losses due to detector dead times, t is the total counting time during the acquisition (in seconds), and F_{att} is the attenuation factor of the attenuator employed¹⁶.

So in this case the previous result, $I_s'''(2\theta)$ is first divided by the efficiency map ε_{xy} and then by the constant factor $t_s \cdot \text{time} \cdot \Phi_0 \cdot (p_x p_y / L^2)$. Here t_s is the sample thickness, time is the counting time corresponding to the sample measurement, p_x and p_y are the horizontal and vertical dimensions of a detector pixel, and L is the sample to detector distance. Thus we obtain the desired result containing the absolute intensity scattered per unit volume as:

$$I(2\theta) = \frac{\left[\frac{I_s(2\theta) - I_{cd}(2\theta)}{T_s(2\theta)T_{sc}(2\theta)} - \frac{I_{sc}(2\theta) - I_{cd}(2\theta)}{T_{sc}(2\theta)} \right]}{t_s \cdot \Delta\Omega(2\theta) \cdot \varepsilon_{xy} \cdot \text{time} \cdot \Phi_0} \text{ (cm}^{-1}\text{)} \quad [\text{Eqn. 4.20}],$$

$$\text{with } \Delta\Omega(2\theta) = \frac{p_x p_y \cos^2(2\theta)}{L^2}.$$

This is the more direct way to obtain the corrected intensity for the sample in absolute units for all the configurations (Low/Middle/High Q) measured and therefore it is proposed as the default option. However the user should take into account that there are some problems associated with the precise measurement of Φ_0 (see e.g. [2]), so the relative precision of the result maybe of the order of 5-10%.

Note that the incident flux is given when the direct beam run is selected to be shown in the plotting window or when the center is calculated. This flux is always given in neutrons per second. However if in the correction window the user has selected the “Use Monitor” option, the time duration of the sample and direct beam (implicit in Φ_0) runs in eqn. 4.20 will be replaced by the monitor values.

B. If the “No scaling” button is toggled, then $I_s'''(2\theta)$ is simply divided by the detector efficiency map:

¹⁶ The attenuation factors used at present for different instruments are given in appendix 3.

$$I_s^{corr}(2\theta) = \left[\frac{I_s(2\theta) - I_{cd}(2\theta)}{T_s(2\theta)T_{ss}(2\theta)} - \frac{I_{ss}(2\theta) - I_{cd}(2\theta)}{T_{ss}(2\theta)} \right] \cdot \left[\frac{1}{\cos^3(2\theta) \cdot \varepsilon_{xy}} \right] \quad [\text{Eqn. 4.21}].$$

In this case the output is a corrected sample intensity, but in arbitrary units.

C. The third possible option is to check the option *Fixed Water Cross Section* in the corresponding menu of calculation options. Then the user has to provide the correct value for $(d\Sigma/d\Omega)_{H_2O,eff}$ in cm^{-1} . This cross section depends on the wavelength employed, but it is also specific to the instrument (see [2]), so the correct value should be given by the instrument responsible. In the ideal case the water and sample measurements would have been performed under the same conditions (same distance and collimation) and then the program performs the following operation:

$$\begin{aligned} I_s^{cor}(2\theta) &= \frac{I_s''(2\theta) \cdot [1/(t_s N_s)]}{I_w''(2\theta) \cdot [1/(t_w N_w)]} \cdot \chi_{H_2O} = \\ &= \frac{\left(\frac{1}{t_s N_s} \right) \left[\frac{I_s(2\theta) - I_{cd}(2\theta)}{T_s(2\theta)T_{ss}(2\theta)} - \frac{I_{ss}(2\theta) - I_{cd}(2\theta)}{T_{ss}(2\theta)} \right]}{\left(\frac{1}{t_w N_w} \right) \left[\frac{I_w(2\theta) - I_{cd}(2\theta)}{T_w(2\theta)T_{sw}(2\theta)} - \frac{I_{sw}(2\theta) - I_{cd}(2\theta)}{T_{sw}(2\theta)} \right]} \cdot \chi_{H_2O} \quad [\text{Eqn. 4.22}]. \end{aligned}$$

When this condition is not applicable¹⁷ the program will estimate the absolute intensity corresponding to the sample by using a scaling factor, F_{sc} . Here there are two possibilities. If the flux at the sample position can be estimated from the direct beam measurements for both the water and the sample, then

$$F_{sc} = \frac{\Phi_s(p_x p_y / L_s^2)}{\Phi_w(p_x p_y / L_w^2)} \quad [\text{Eqn. 4.23}].$$

Otherwise

$$F_{sc} = \left(\frac{C_w L_w}{C_s L_s} \right)^2 \quad [\text{Eqn. 4.24}],$$

where C_s and C_w are the collimations employed in both measurements.

In the first case we have:

¹⁷ This is always the case for the low-Q run (as normally water is not measured at the large detector distance configuration) and also for the high-Q run if water has been measured using only the middle-Q configuration. However it can also happen that the water run conditions do not correspond to any of the sample runs, so in this case the three configurations will be rescaled.

$$I_s^{corr}(2\theta) = \frac{I_s'''(2\theta) \cdot [1/(t_s N_s)]}{I_w'''(2\theta) \cdot [1/(t_w N_w)]} \cdot \left(\frac{\chi_{H_2O}}{F_{sc}} \right) =$$

$$\frac{\left(\frac{1}{t_s N_s} \right) \left[\frac{I_s(2\theta) - I_{Cd}(2\theta)}{T_s(2\theta) T_{es}(2\theta)} - \frac{I_{es}(2\theta) - I_{Cd}(2\theta)}{T_{es}(2\theta)} \right]}{\left(\frac{1}{t_w N_w} \right) \left[\frac{I_w(2\theta') - I_{Cd}(2\theta')}{T_w(2\theta') T_{ew}(2\theta')} - \frac{I_{ew}(2\theta') - I_{Cd}(2\theta')}{T_{ew}(2\theta')} \right]} \cdot \left(\frac{\Phi_w \Delta \Omega_w}{\Phi_s \Delta \Omega_s} \right) \cdot \chi_{H_2O} \quad [\text{Eqn. 4.25}].$$

This result is correct, but it will suffer from the same problems related with the precise measurement of the neutron flux mentioned before. In the second case, where Φ_s or Φ_w or both are not available, we have:

$$I_s^{corr}(2\theta) = \frac{I_s'''(2\theta) \cdot [1/(t_s N_s)]}{I_w'''(2\theta) \cdot [1/(t_w N_w)]} \cdot \left(\frac{\chi_{H_2O}}{F_{sc}} \right) =$$

$$\frac{\left[\frac{I_s(2\theta) - I_{Cd}(2\theta)}{T_s(2\theta) T_{es}(2\theta)} - \frac{I_{es}(2\theta) - I_{Cd}(2\theta)}{T_{es}(2\theta)} \right]}{\left[\frac{I_w(2\theta') - I_{Cd}(2\theta')}{T_w(2\theta') T_{ew}(2\theta')} - \frac{I_{ew}(2\theta') - I_{Cd}(2\theta')}{T_{ew}(2\theta')} \right]} \left(\frac{t_w N_w \Delta \Omega_w}{t_s N_s \Delta \Omega_s} \right) \left(\frac{C_s L_s}{C_w L_w} \right)^2 \chi_{H_2O} \quad [\text{Eqn. 4.26}].$$

D. The last possibility is that the user has selected one of the previous options, but the required information to do the full treatment is missing. In this case the program will try to find the best solution achievable with the available information. Possible situations are:

- i. There is no water measurement: In this case the detector efficiencies cannot be calculated, so the treatment is done assuming $\epsilon_{xy}=1$ for all the detector pixels. If the absolute calibration using water has been requested, the program will use instead the flux obtained from the direct beam measurement to compute the absolute intensity.
- ii. If any background or absorbent measurements are missing, the program will proceed without doing the corresponding subtractions.
- iii. If a transmission run is missing the user must provide a reasonable value in the corresponding Tr.Wvalue or Tr.value cell in the spreadsheet. Otherwise the message “? Bad Transmissions, use Transmission menu or enter a value manually” will appear.
- iv. The default calculation (using the neutron flux) is required, but the incident flux cannot be calculated for one or several configurations. This should not happen normally, but if for any reason the distance and/or collimation corresponding to the sample measurement are not the same than those of the direct beam measurement, then Φ_0 cannot be calculated. It also could happen that a direct beam measurement is missing and the center has been set manually. In this case, the program will use

the water measurement to do the absolute calibration (case C). The difficulty now is that the correct value for $\chi_{\text{H}_2\text{O}}$ is not given. If the incident flux corresponding to the water measurement can be estimated (i.e. there exists a direct beam measurement done with the same conditions), then $\chi_{\text{H}_2\text{O}}$ is calculated as¹⁸:

$$\chi_{\text{H}_2\text{O}} = \left\langle \left[\frac{I_w(2\theta) - I_{cd}(2\theta)}{T_w(2\theta)T_{sw}(2\theta)} - \frac{I_{sw}(2\theta) - I_{cd}(2\theta)}{T_{sw}(2\theta)} \right] \left(\frac{1}{t_w \Phi_w \Delta\Omega(2\theta) \cdot \text{time}} \right) \right\rangle$$

[Eqn. 4.27].

Otherwise the default value $\chi_{\text{H}_2\text{O}} = 1$ is used.

- v. Finally, if the neutron flux cannot be estimated and there is no water measurement, the program will return the sample corrected data in arbitrary units (case B).

9. The Q-resolution is estimated using the following equation [3]:

$$\sigma(Q)^2 = Q^2 \left(\frac{1}{2\sqrt{2\ln 2}} \frac{\Delta\lambda}{\lambda} \right)^2 + \left[\left(\frac{4\pi}{\lambda} \right)^2 - Q^2 \right] \sigma(\theta)^2 \quad [\text{Eqn. 4.28}].$$

where $\sigma(Q)$ is the standard deviation of the Gaussian distribution representing the resolution in Q, $(\Delta\lambda/\lambda)$ is the full width at half maximum of the wavelength distribution (read from the numor parameters or set to 0.1 otherwise), and $\sigma(\Theta)$ is the standard deviation of the Gaussian used to represent the angular distribution of the incident beam. The later is obtained from a fit of the direct beam as:

$$\sigma(\Theta) = \tan^{-1} \left[\frac{1}{2} \frac{1}{2\sqrt{2\ln 2}} \frac{\langle \text{FWHM}_{xy} \rangle}{L} \right] \quad [\text{Eqn. 4.29}],$$

where L is the sample to detector distance and $\langle \text{FWHM}_{xy} \rangle$ is the average beam size. This is computed as the average of the two FWHMs obtained from the fit of the horizontal and vertical beam profiles to two Gaussians,

Figure 4.3 shows an example of the resolution curves obtained on D11 for three typical configurations.

¹⁸ Whenever possible, this calculation is always done and the result is returned in the case Fixed Water Cross Section, except if this option has been selected and a value entered manually

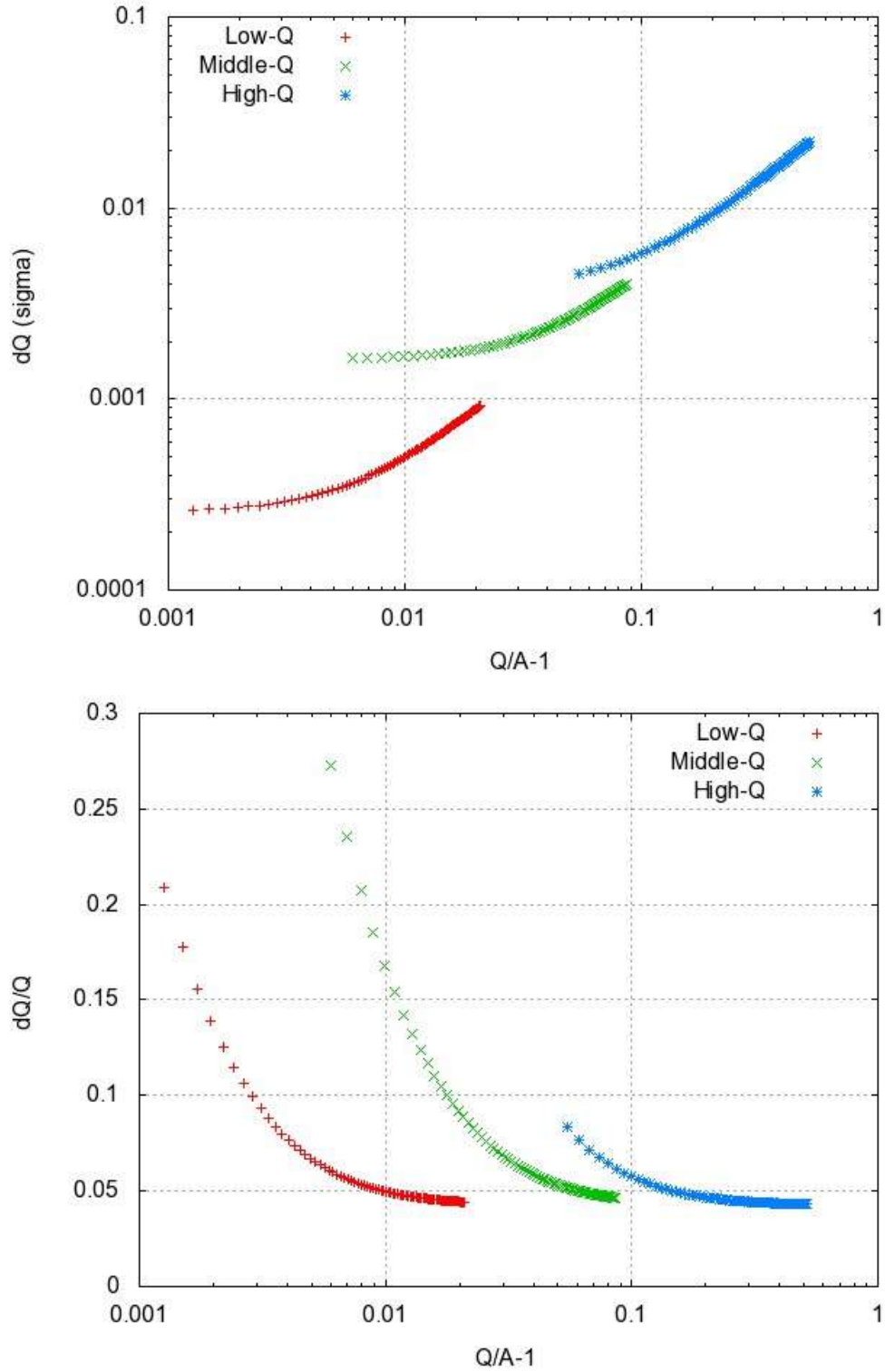


Figure 4.3: Resolution curve, $\sigma(Q)$ (up) and $\sigma(Q)/Q$ (bottom), for $\lambda=6\text{\AA}$ and three typical configurations of D11: Low-Q ($L = 34$ m, collimation = 34 m, $\sigma(\Theta) = 0.000123$ rad), Middle-Q ($L = 8$ m, collimation = 8 m, $\sigma(\Theta) = 0.000770$ rad), and High-Q ($L = 1.2$ m, collimation = 5.5 m, $\sigma(\Theta) = 0.00186$ rad).

5. Anisotropic data

The data correction procedure described in the previous section is applied to the 2D data, so the corrected (non integrated) data can be exported for further analysis using the Export menu. But it is also possible to perform different anisotropic integrations using directly Sans spreadsheet.

In order to do this, the option GROUP Mode = By Sectors has to be selected in the Treatment Options menu. Once this is done, the option Sector Mode will become available in the same menu. Select Radial integration symmetrical if there are two planes of symmetry in the data such that $I(x)=I(-x)$ and $I(y)=I(-y)$, or otherwise use the Radial integration non-symmetric option. The total integration option can be used to compute only the integrated intensity in each region. Once this is done, the “Defining Sectors” window will appear (Fig. 5.1). In this window the user can define the number of different sectors needed and their inner and outer radius. Note that each sector has a mirror image, so choosing 2 sectors you will sketch 4 regions in the image. In the case of the symmetric option, the mirror sectors would be averaged together giving two $I(Q)$ curves, but in the non-symmetric case they would be treated separately giving four different $I(Q)$ curves.

The sectors can be rotated using the “Rotation 0.1 deg” bar, which rotates all of them by the angle given (see Fig. 5.2 where a rotation of 45° has been applied). When only 2 sectors have been defined, the “Single rotation” bar allows rotating the second one without displacing the first one. Finally the “Opening” bar allows selecting the angular size of the vectors defined. The “Squared Sectors” option below the Center line can be employed to define some trapezoidal or roughly rectangular regions (Fig. 5.3). The “Surf” button can be employed to get a larger surface image of the data as shown in Fig. 5.4, which can be useful in some cases to help in defining the right integration regions.

Once the sectors have been appropriately defined the Treat option must be used to correct the data and perform the required integrations. The radial integration performed in each independent sector will appear as a different line in the results window (Fig. 5.5). The line contains the numor, the sample number, the standard keyword to indicate low (pL), middle (mM) or large (gH) Q configuration and the corresponding sector. For example, if two non-symmetric sectors are defined and they are not rotated, the output will contain 4 results named as XXX.Sect000.0, XXX.Sect090.0, XXX.Sect180.0, and XXX.Sect270.0 + the keyword unS (see Fig. 5.4). In the same example, if the symmetric option is applied the output will consist of only 2 results XXX.Sect180.0, and XXX.Sect270.0 + the keyword Sym.

The different results in the Results window can be manipulated and exported as usual.

Finally note that if several Q-configurations are employed the user must define the sectors for the three of them (Low, Middle and High-Q) before launching the treatment.

Another possibility in the Sector mode menu consists in selecting “Total integration” (either symmetrical or not) and then using the rocking button in the sectors window to obtain the total number of counts in one or several detector regions as a function of a given parameter: sample number, time, temperature, etc. (see the example in next section).

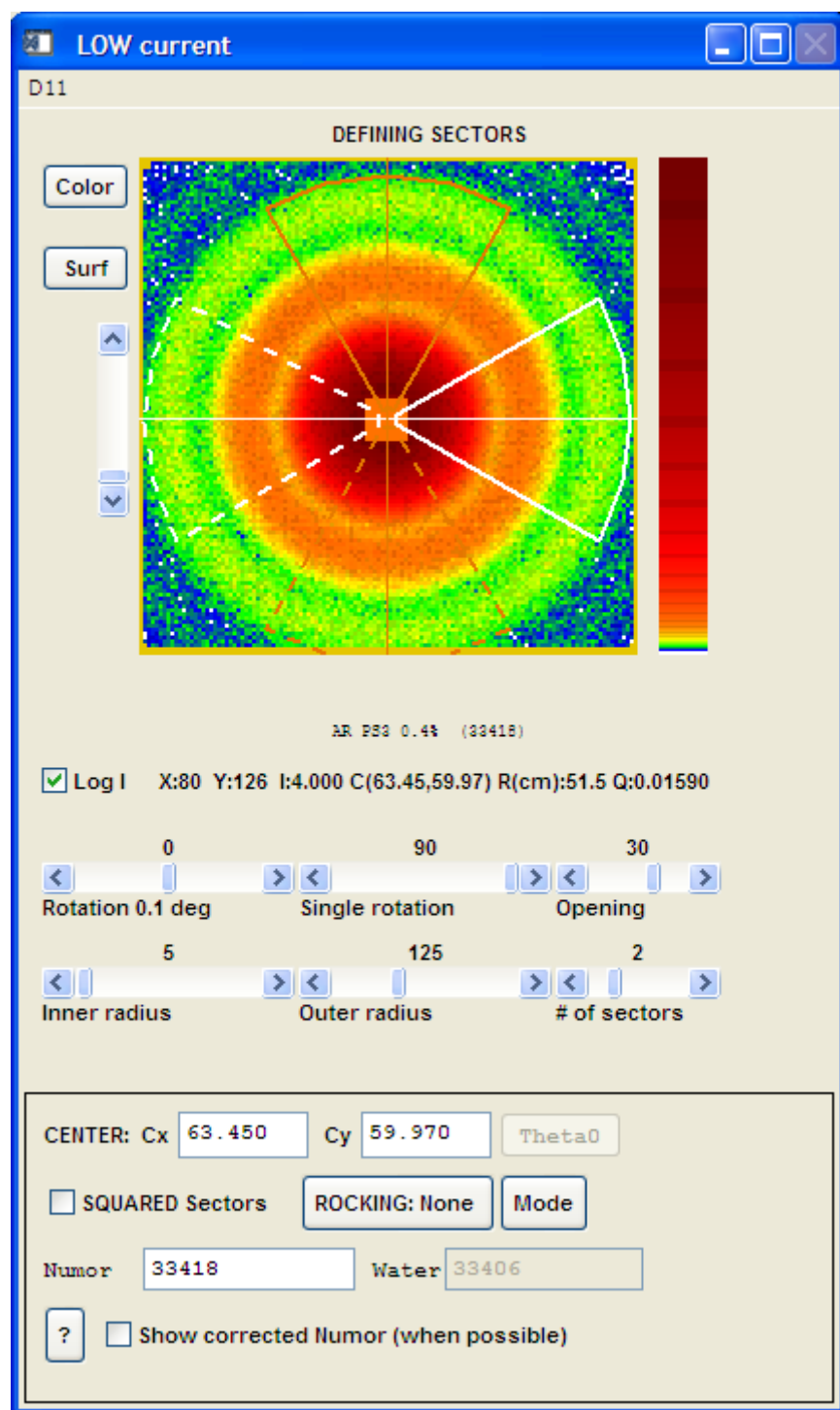


Figure 5.1: Window allowing defining different sectors. In the example shown here two sectors are defined (and shown with different colors in the plot) and the radial integration is non-symmetric (shown with the continuous and broken lines), giving a total of four different regions where the radial integration will be performed. If the symmetric option would have been chosen then the broken lines would have been replaced by a continuous line and the integration would be performed over only two different regions (those delimited by the white and orange lines).

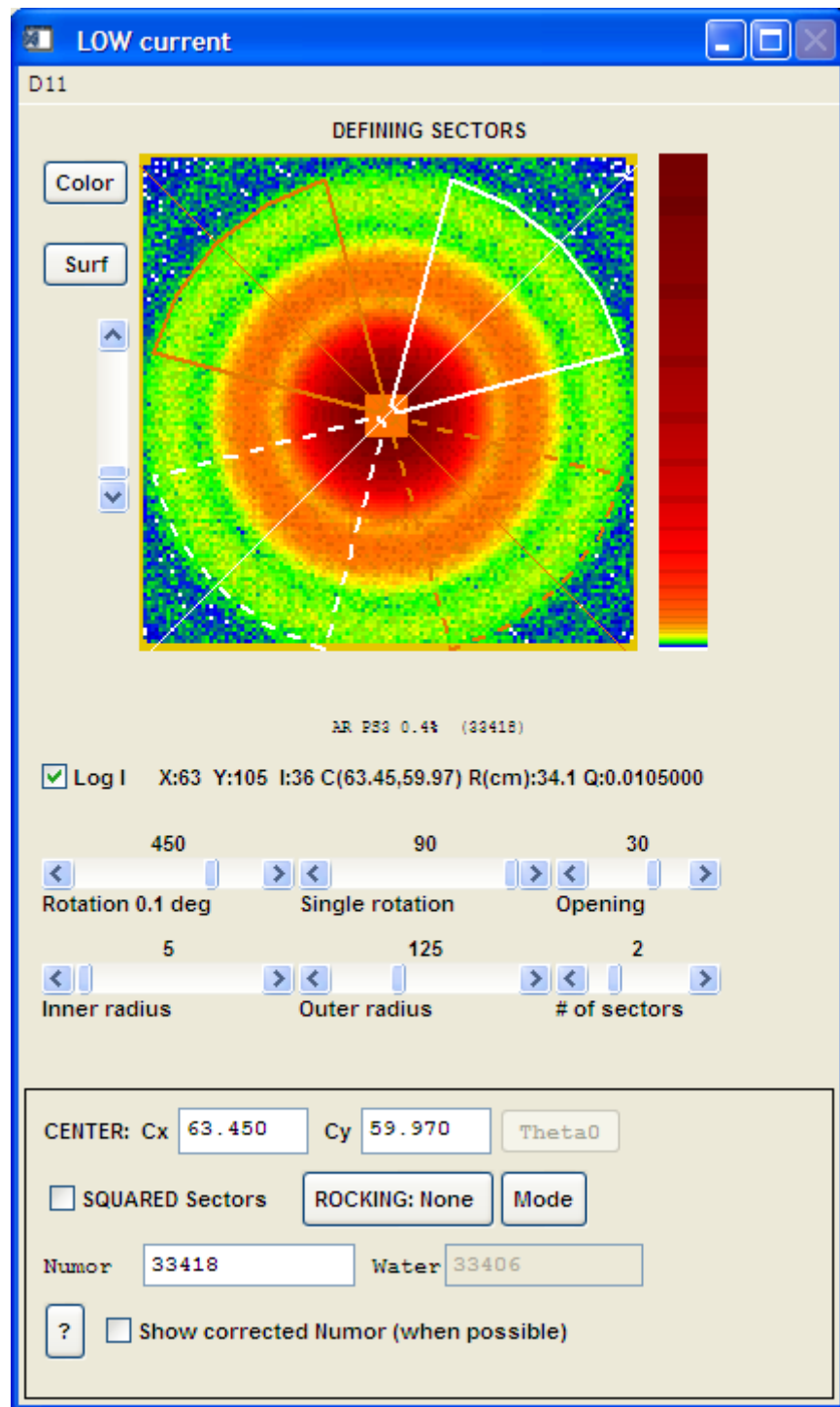


Figure 5.2: The size and orientation of the selected regions can be changed using the sliding bars available in the sectors window.

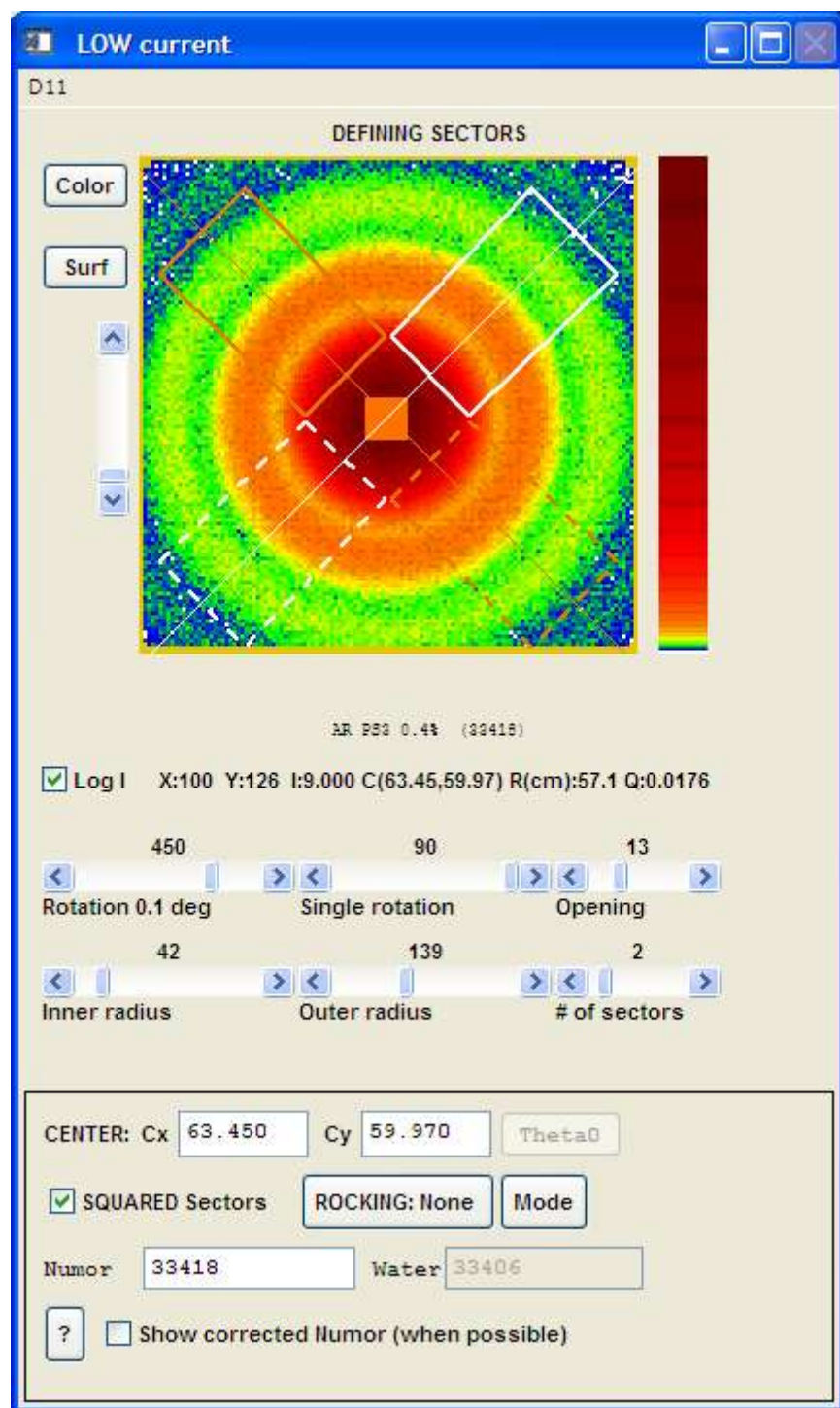


Figure 5.3: The shape of the sectors can be changed to square-like by toggling the “Squared Sectors” option.

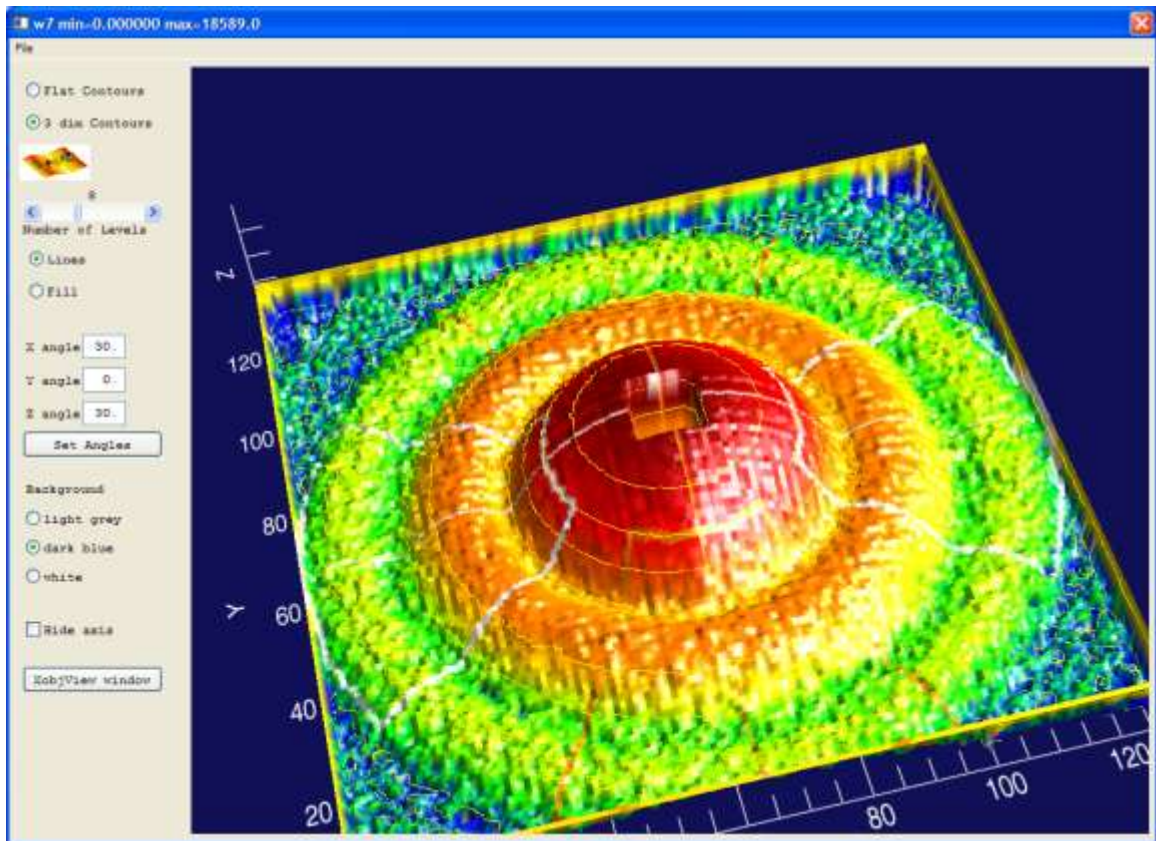


Figure 5.4: Surface image showing the raw data and the sectors actually defined.

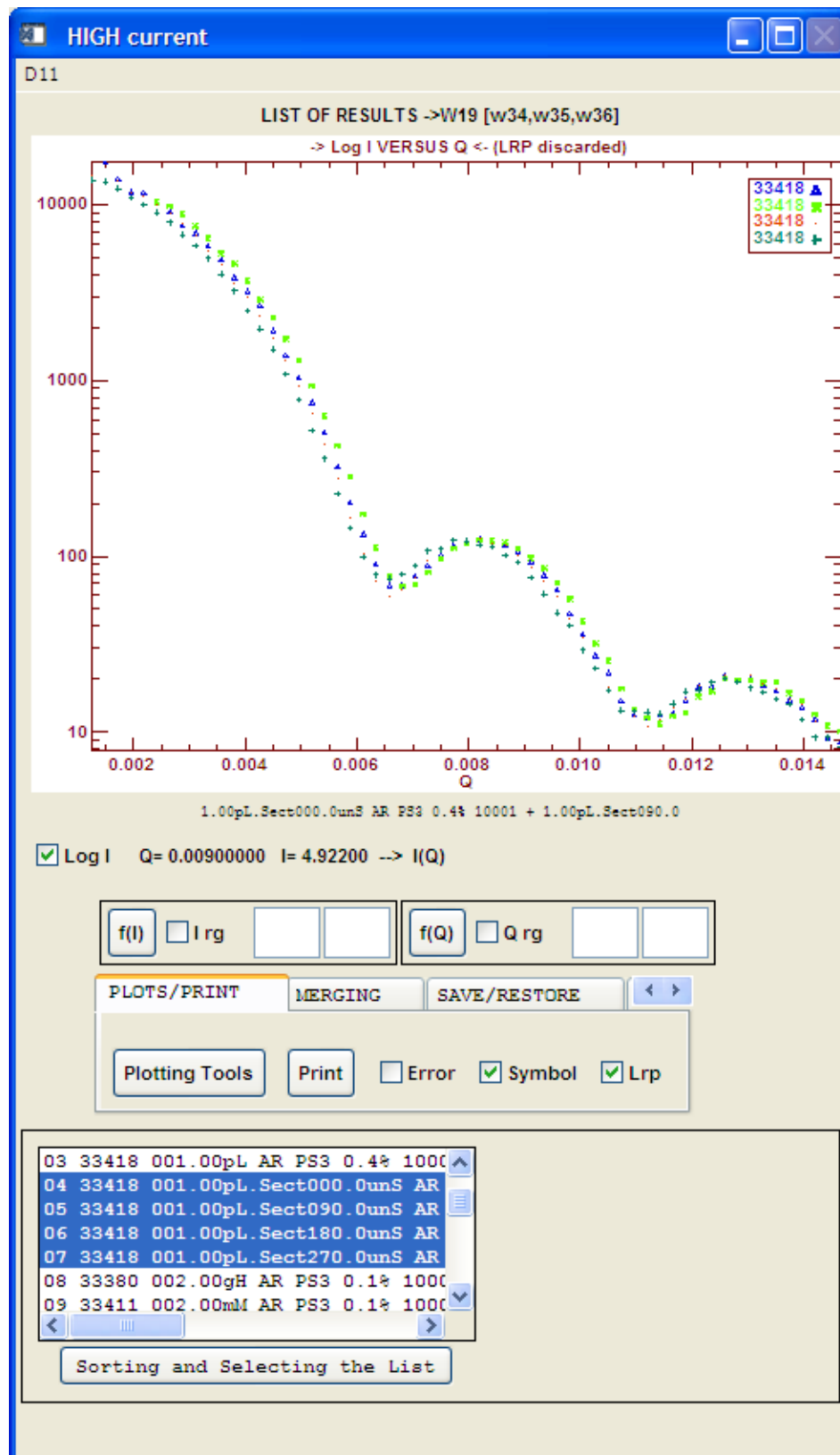


Figure 5.5: Results window showing the radially integrated curves for the example case shown in figure 5.1.

6. Kinetic data

Sans spreadsheet can read directly a kinetic numor, i.e. a numor file containing more than one acquisition. In this case each of the data sets contained in the numor will be treated independently and the list of results will contain as many lines as the number of acquisitions contained in the kinetic file. The resulting $I(Q)$ data can be treated and visualized as previously explained, but they can also be plotted as a 3D surface. Such representation is obtained from the “Plotting Tools” menu shown in figure 6.1 and in the 3D plot the y axis may correspond either to the run number or to the run time since the starting time. Figure 6.2 provides an example of such plot.

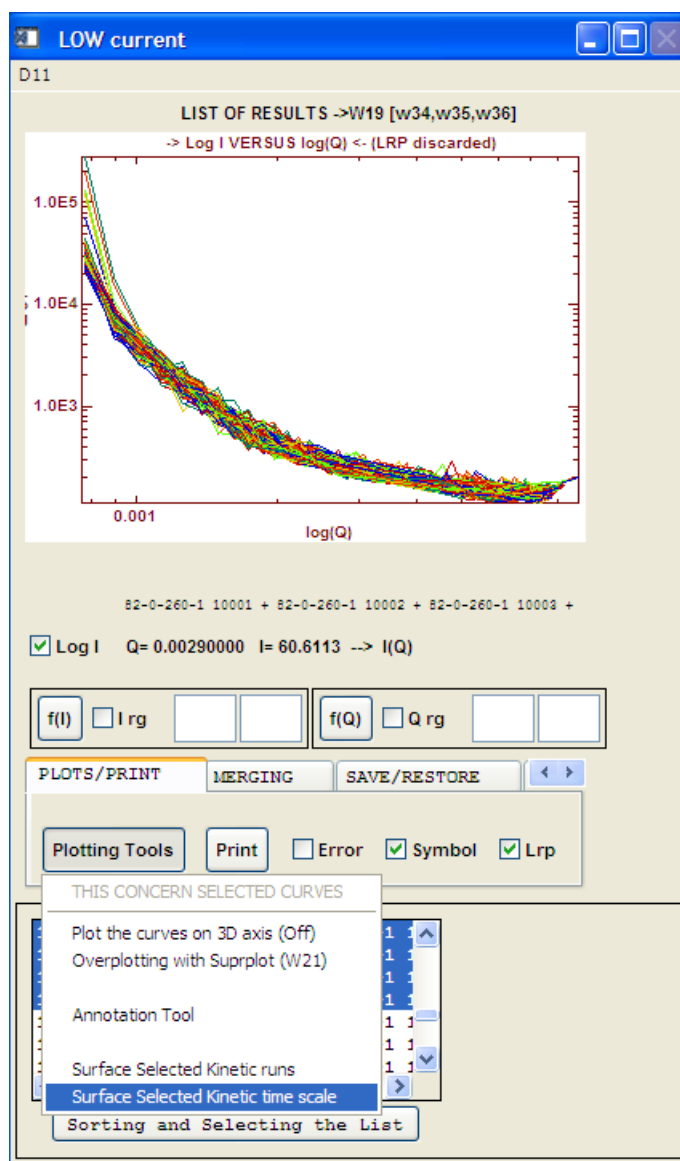


Figure 6.1: Options to plot a series of (kinetic) curves in 3D.

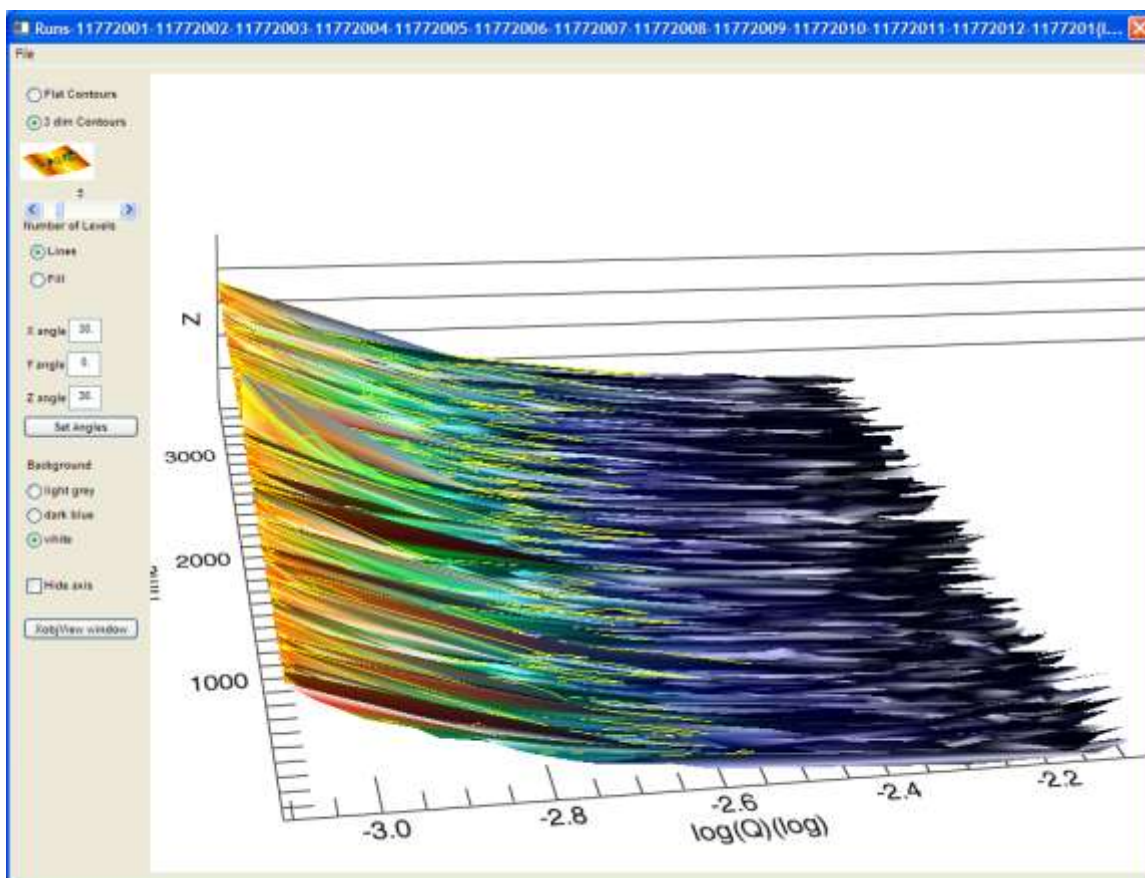


Figure 6.2: Example of a 3D plot.

For the data treatment procedure, kinetic runs are treated in the same way as if they were different samples. The only difference is that all of them will be associated to the same transmission run and therefore they will all have the same transmission. A similar result is obtained if a series of numbers is given in one cell employing the syntax " $N_1 : N_{last}$ ". It is even possible to combine in a single cell kinetic and normal runs, for example using the following syntax: " $N_{kin} , N_1 : N_{last}$ "!

The rocking option mentioned in the previous section can be used to explore rapidly any change in the scattering intensity with sample number, time or any other appropriate variable. As an example figure 6.3 shows a simple table containing a single sample that evolves in time. The changes can be appreciated easily using the slide bar of the plotting window (Fig. 6.4). And if a single sector is defined together with the total integration option and the "ROCKING: Times" selection as shown in Fig. 6.4 we will obtain in the list of results a single curve of the total scattering intensity as a function of time (Fig. 6.5).

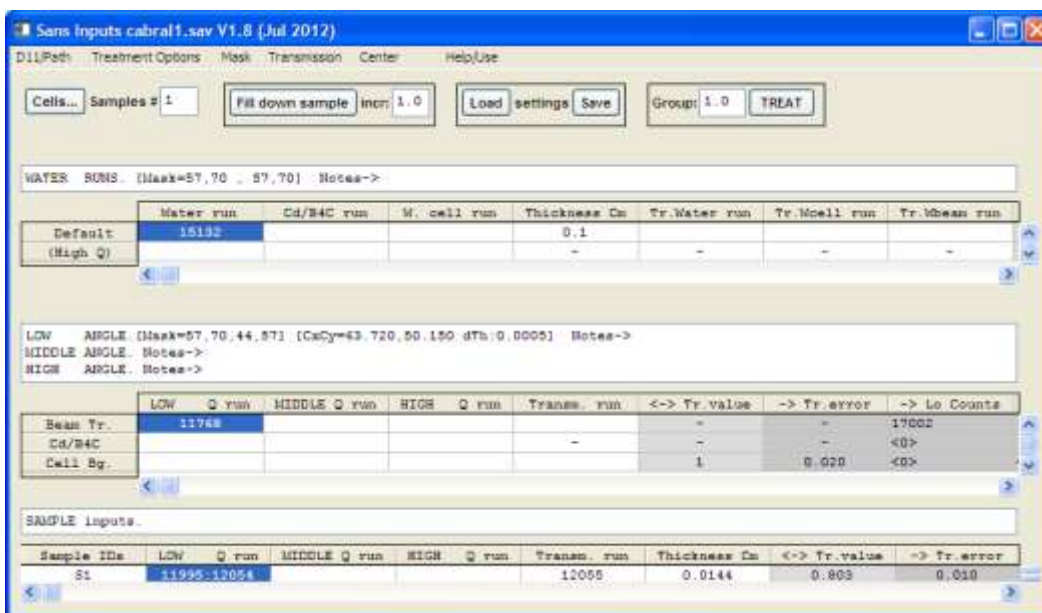


Figure 6.3: Simple table showing a series of numors corresponding to consecutive measurements on the same sample and read into a single cell.

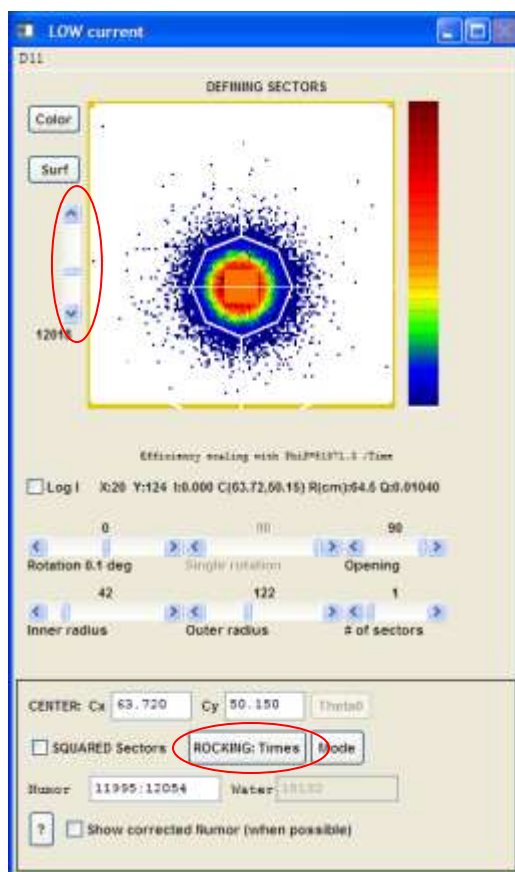


Figure 6.4: Plotting window showing a data snapshot, the sliding bar to navigate between the data sets and the rocking integration option.

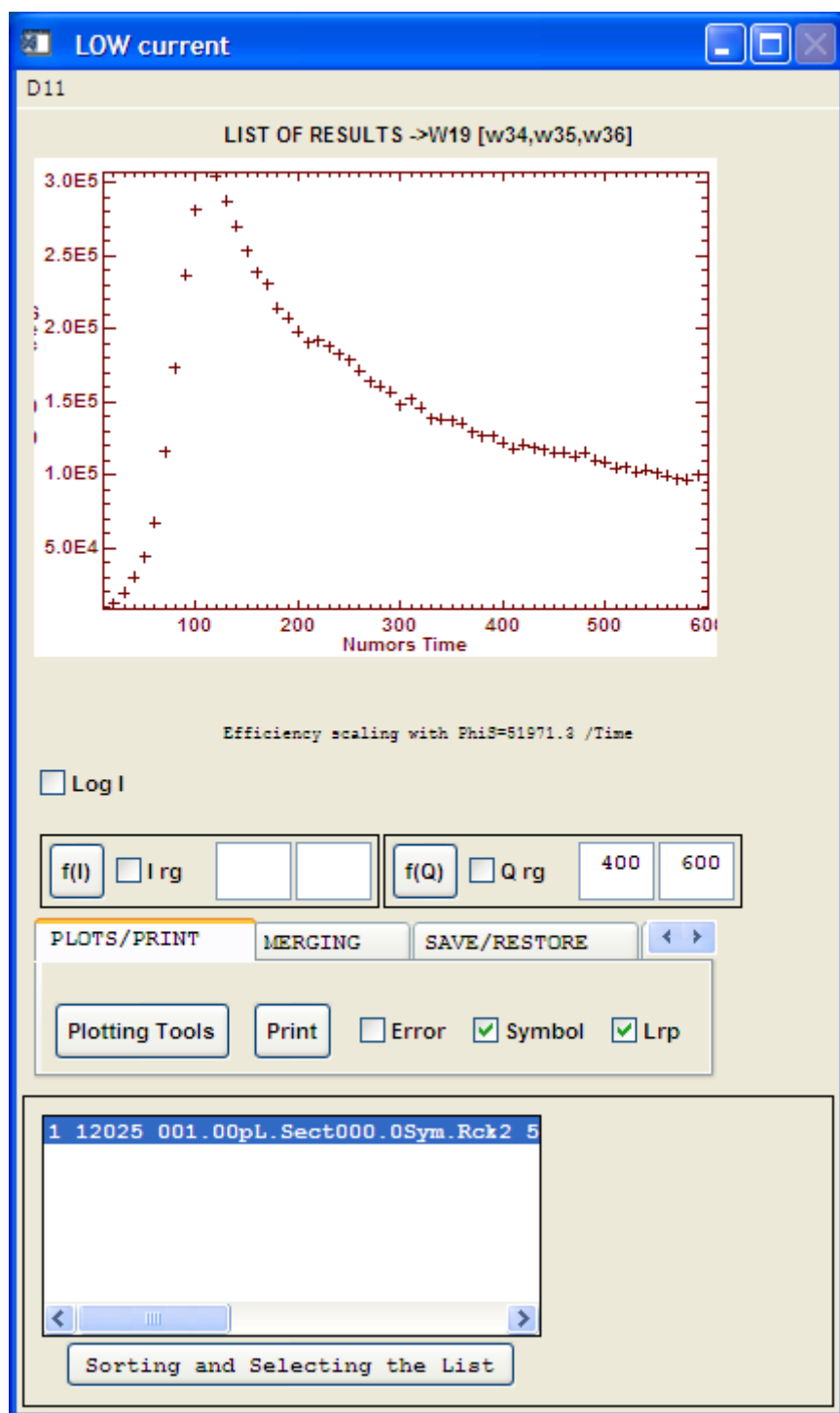


Figure 6.5: Total scattering intensity in the integration region defined by the sector drawn in figure 6.2 as a function of measuring time.

7. D16

Under development ...

8. Final remarks and acknowledgments

Sans spreadsheet has evolved over several years in order to hopefully produce a reliable and user friendly tool that will help the ILL users to reduce efficiently their SANS data. By now the code has been tested in many different circumstances and it appears to be reasonably robust, providing consisting results with the other codes employed at the ILL to treat the data from D11 and D22 whenever equivalent conditions are used. However the code is in constant evolution following the continuous requests from users and instrument responsables and we cannot discard the possibility that some particular combinations or some new additions may result in an unexpected behavior or a wrong result. In this case please write to any of us (richard@ill.eu or gonzalez@ill.eu).

Finally we would like to help the input of all the Large Scale Structures group at the ILL, and in particular the active involvement and the useful criticisms to improve the program from Isabelle Grillo, Bruno Deme, Ralf Schweins and Peter Lindner.

9. Appendixes

1. Correction function (Qdep) for D22

In the case of D22, the correction applied at present depends on the horizontal scattering angle, $2\Theta_x$, and takes the following form:

$$I^{corr}(2\theta_x) = I(2\theta_x) \cdot [1 + F(2\theta_x) - F(0)] \quad [\text{Eqn. 4.16}],$$

with

$$F(2\theta_x) = A \exp[(-4 \ln 2)(2\theta_x - B)^2 / C^2], \quad \text{if } |2\theta_x| < B$$

$$F(2\theta_x) = A \quad \text{if } |2\theta_x| \geq B \quad [\text{Eqn. 4.17}].$$

A first fit to a limited set of water measurements gave the following parameters: $A = 0.140$, $B = 0.588$ rad, and $C = 0.414$ rad. In Grasp, a 5th degree polynomial is used to correct for the parallax effect in D22. As shown in figure 4.1, in the range $2\Theta_x < 35^\circ$ a quite close correction can be obtained using the previous equation together with the following parameters: $A = 0.153$, $B = 0.698$ rad, and $C = 0.630$ rad.

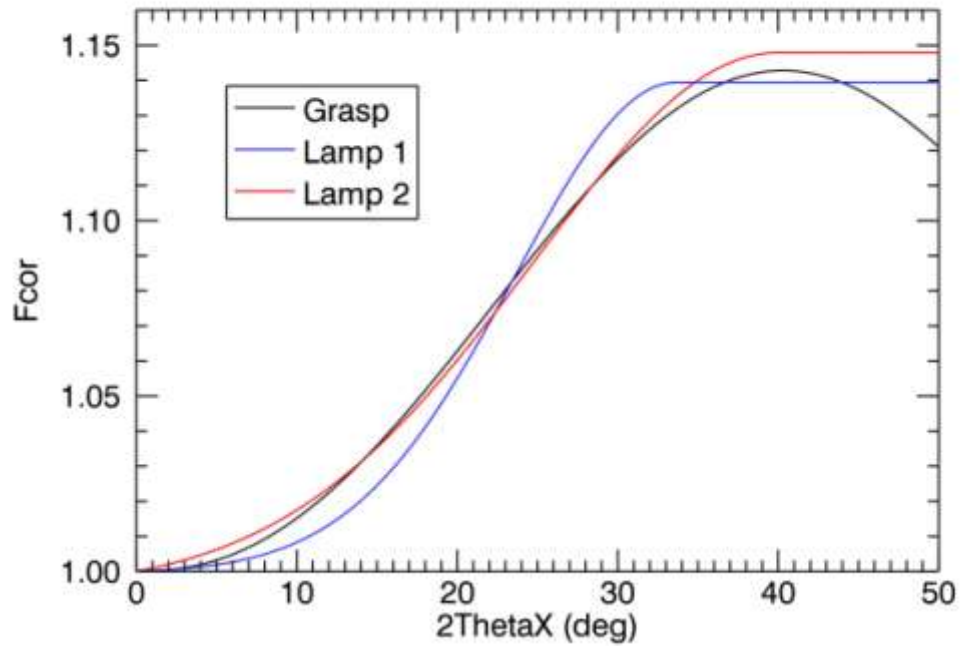


Figure 4.1: Comparison of the curves employed in Lamp and Grasp to correct the parallax effect of the D22 detector. The curve named Lamp1 is obtained with the first

set of parameters (A=0.140, B=0.588, C=0.414), while the curve Lamp2 corresponds to the second set (A=0.153, B=0.698, C=0.630).

2. Correction function (Qdep) for D11

In the case of D11 the dependence observed in several water measurements was reproduced using eqn. 4.16 with this function:

$$F(2\theta, r) = \cos^2\left(\frac{2\theta^3}{2L}\right) \left[1 - 0.1\left(\frac{r}{r_{max}}\right)\right] \quad [\text{Eqn. 4.18}],$$

where 2θ and r correspond to the angle and distance to the beam center of each detector pixel, L is the sample to detector distance, and r_{max} is the maximum value of r .

An alternative function that has also been used to model the angle dependence of the water measurements is the following one:

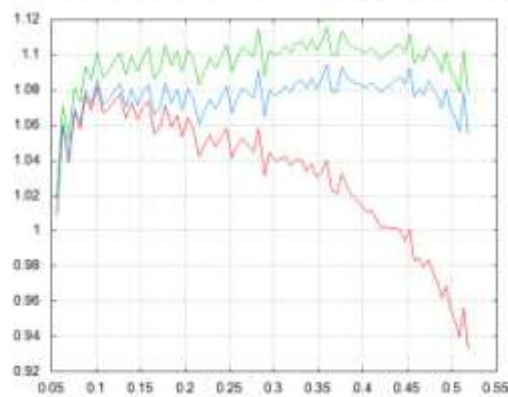
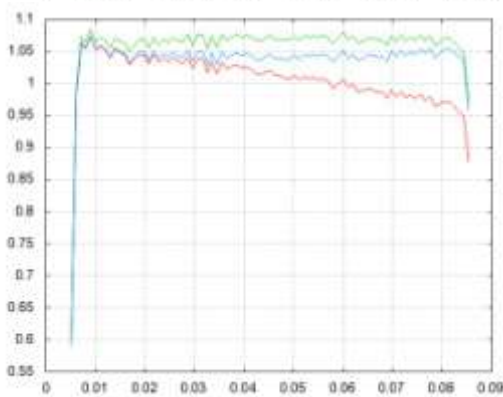
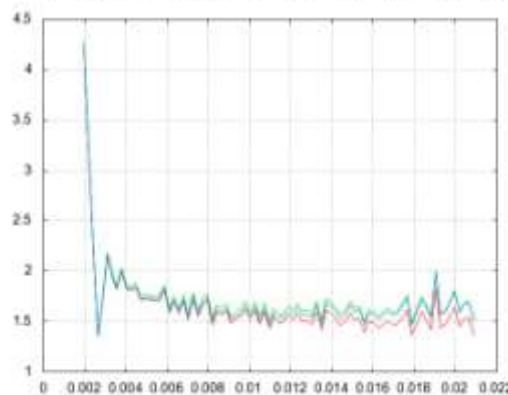
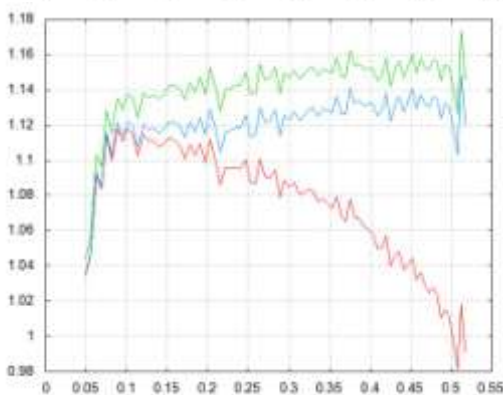
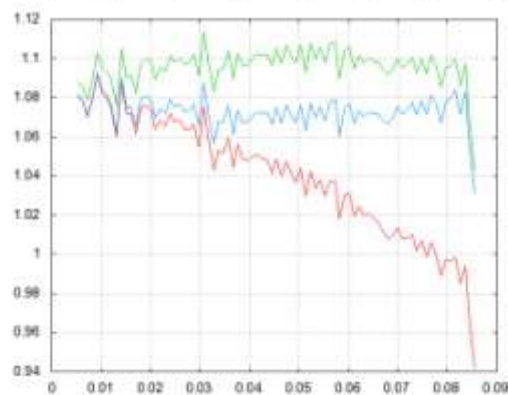
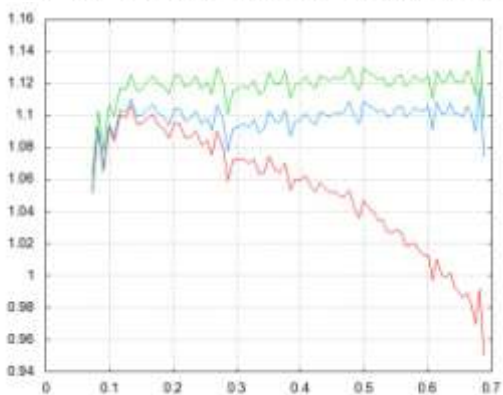
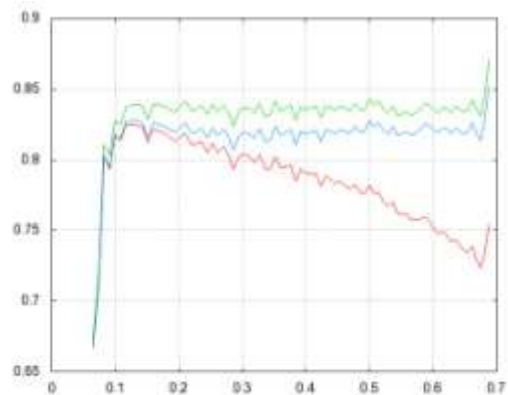
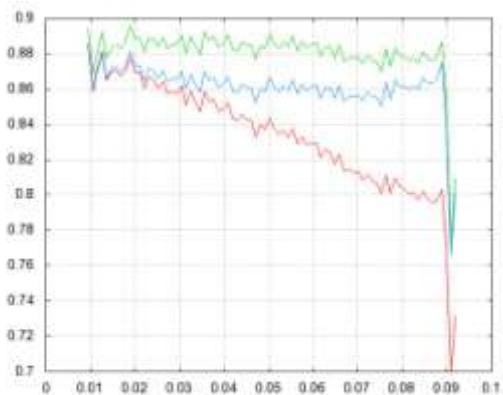
$$F(2\theta) = 1 + A \tan^2(2\theta) + B L^2 \tan^2(2\theta) \quad [\text{Eqn. 4.19}],$$

with $A = -0.10$ and $B = -0.20$.

The water runs employed to obtain those corrections are given in table 4.1, where the measurement conditions (wavelength, detector distance, and collimation) are also indicated. The effect of this correction in the final water curves is shown in figure 4.2.

	Date	λ	L	Coll	Direct Beam	Blocked Beam	Empty Cell	H ₂ O
1	Oct 2009	4.5	10.	10.5	25621	25619	25617	25616
2	Oct 2009	4.5	1.2	16.5	25626	25630	25628	25627
3	Sep 2011	4.5	1.2	10.5	17076	17153	17075	17074
4	Sep 2010	6.0	8.0	8.0	7308	7311	7310	7309
5	Sep 2010	6.0	1.2	10.5	7307	7306	7305	7304
6	Sep 2010	6.0	34.	34.0	7551	7529	7528	7527
7	Sep 2010	6.0	8.0	8.0	7526	7535	7534	7533
8	Sep 2010	6.0	1.2	5.5	7525	7547	7546	7545
9	Sep 2011	6.0	1.2	10.5	16994	16993	16992	16991
10	Nov 2011	6.0	8.0	8.0	28401	28398	28397	28396
11	Nov 2011	6.0	1.2	5.5	28393	28404	28403	28402
12	Nov 2011	6.0	1.2	8.0	28211	28208	28220	28231
13	Nov 2009	10.0	8.0	5.5	31686	31681	31678	31676+31677
14	Nov 2009	10.0	1.2	2.5	31695	31700	31697	31696
15	Nov 2011	13.0	4.0	4.0	28212	28217	28218	28230
16	July 2011	13.0	4.0	4.0	12098	12095	12094	12093

Table 4.1: Water runs employed in determining the Q-dependent correction for D11.



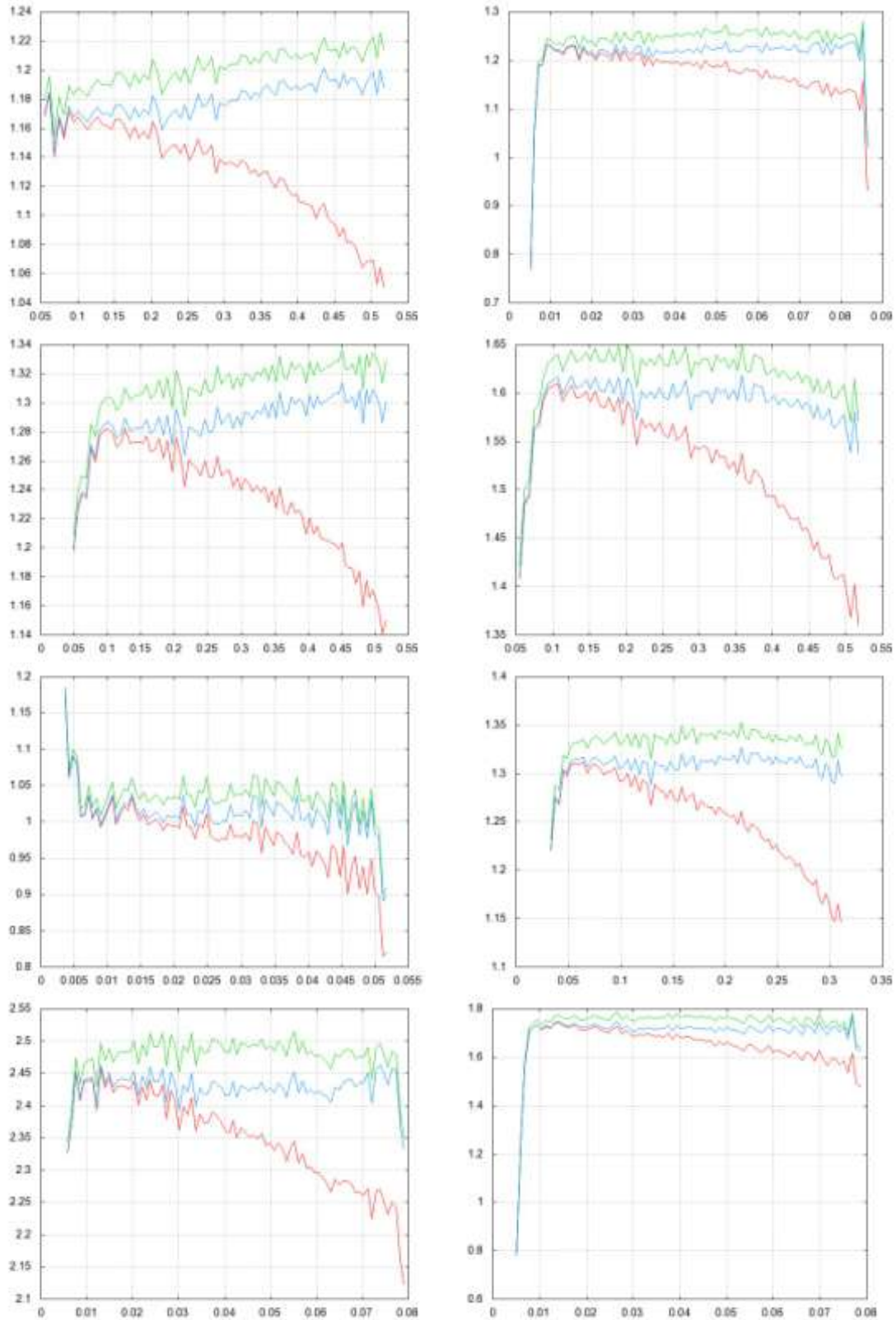


Figure 4.2: $I(Q)$ for the water measurements given in table 4.1 when no instrument correction is applied (red curve), or applying the corrections given by Eqn. 4.18 (green curve) and Eqn. 4.19 (blue curve)

3. Table of attenuation factors

Instrument	Attenuator 1	Attenuator 2	Attenuator 3
D11	289.017	917.431	2840.91
D22	147	902	2874
D16	10	100	1000
BRISP	-	-	-

At present SANS spreadsheet uses constant attenuation factors. A future development may consist in including the wavelength and collimation dependence of those factors, as done already in Grasp for D22.