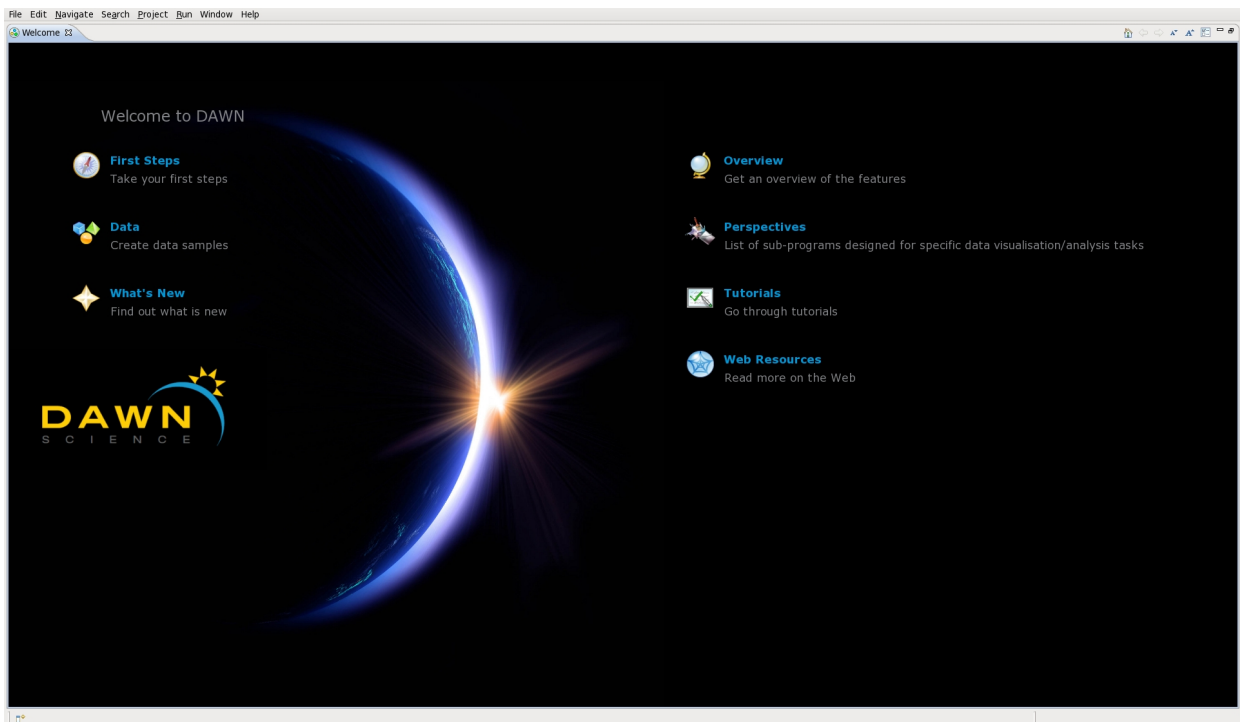


Tutorial on SAXS data reduction in DAWN

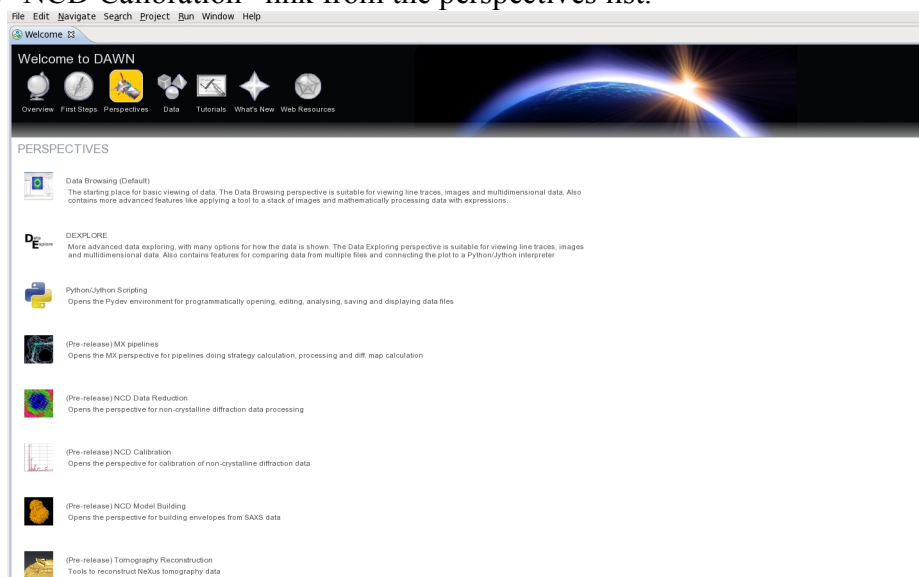
S4SAS Workshop, Diamond Light Source, July 2014

1. Open a terminal window. On a command line type :

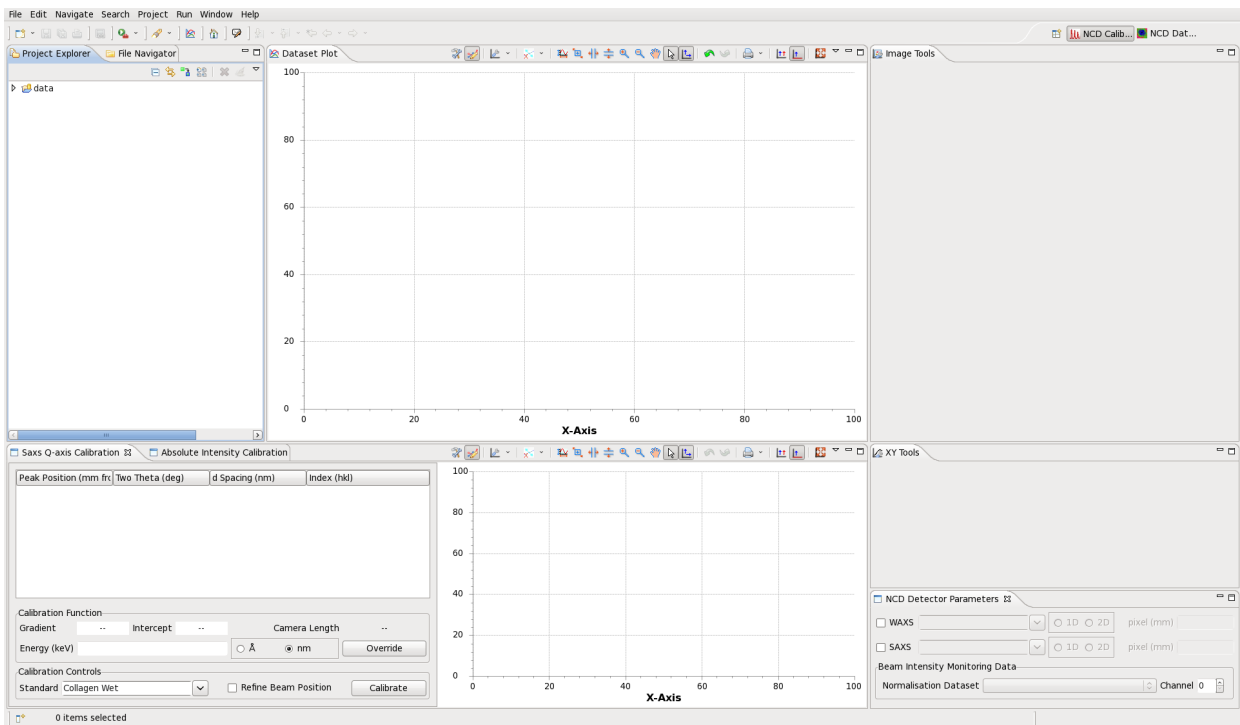
```
module load dawn  
dawn -data /some/place/DAWN_S4SAS
```
2. On the DAWN Welcome screen select “Perspectives” link.



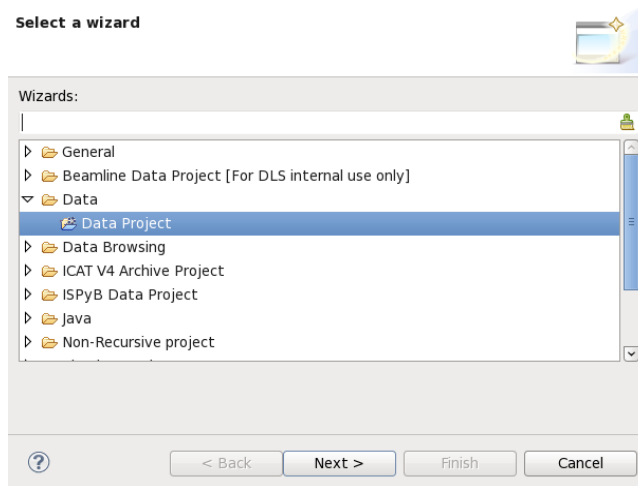
3. Select “NCD Calibration” link from the perspectives list.



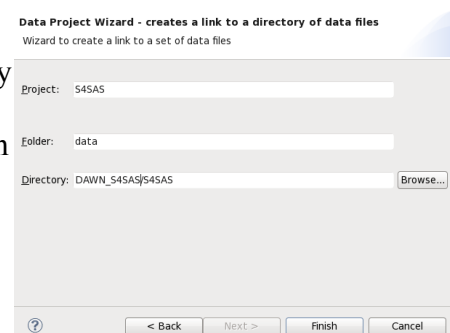
- On the “NCD Calibration” perspective you should see one project in the “Project Explorer” view: data.



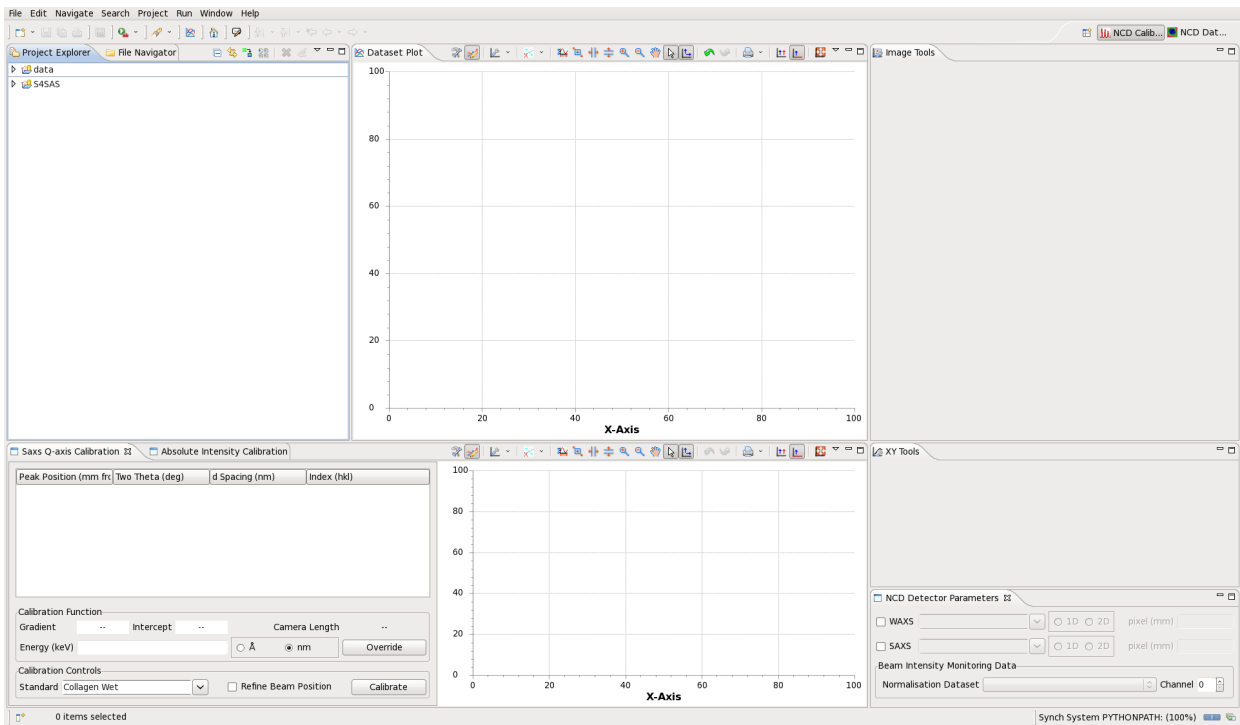
- Right-click inside the “Project Explorer” view and select New -> Project... and select Data -> Data Project...



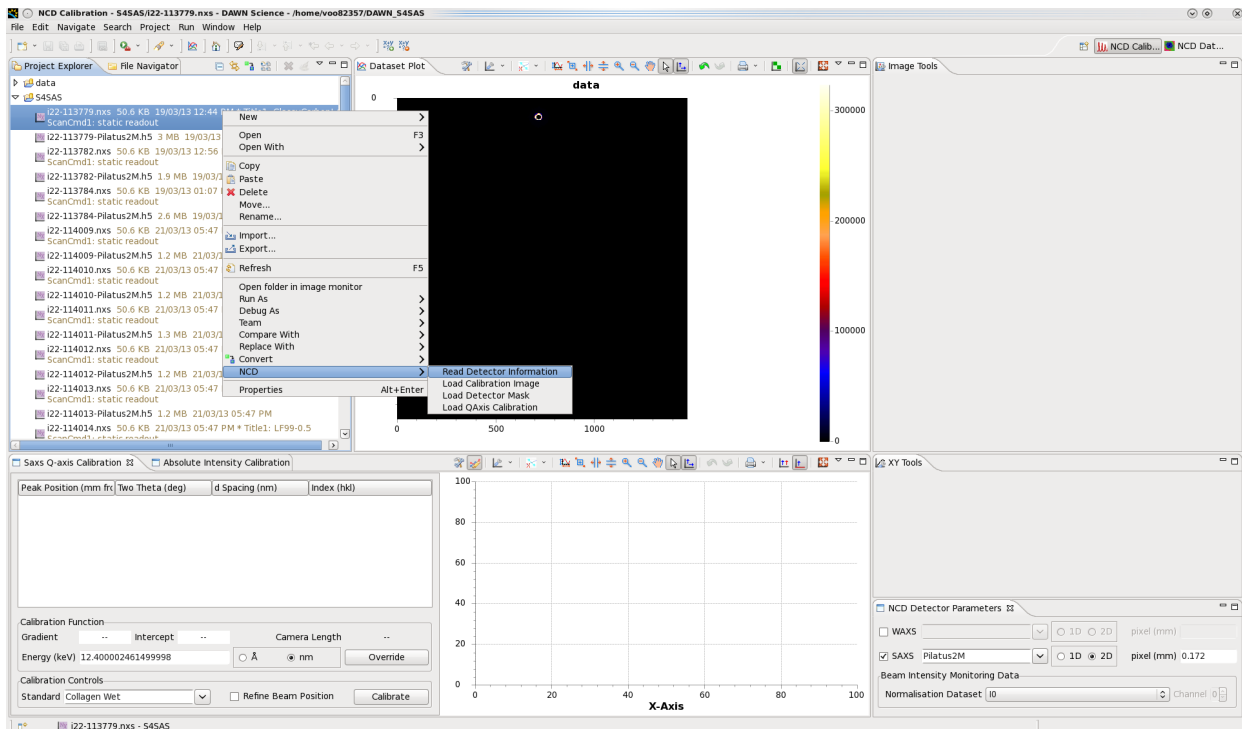
- On the following page specify project name. In the Directory field specify the location of “S4SAS” directory that is inside the DAWN_S4SAS workspace and press “Finish”. You can use “Browse...” button to look through file system.



7. On the “NCD Calibration” perspective you should now see two projects in the “Project Explorer” view: data and S4SAS.

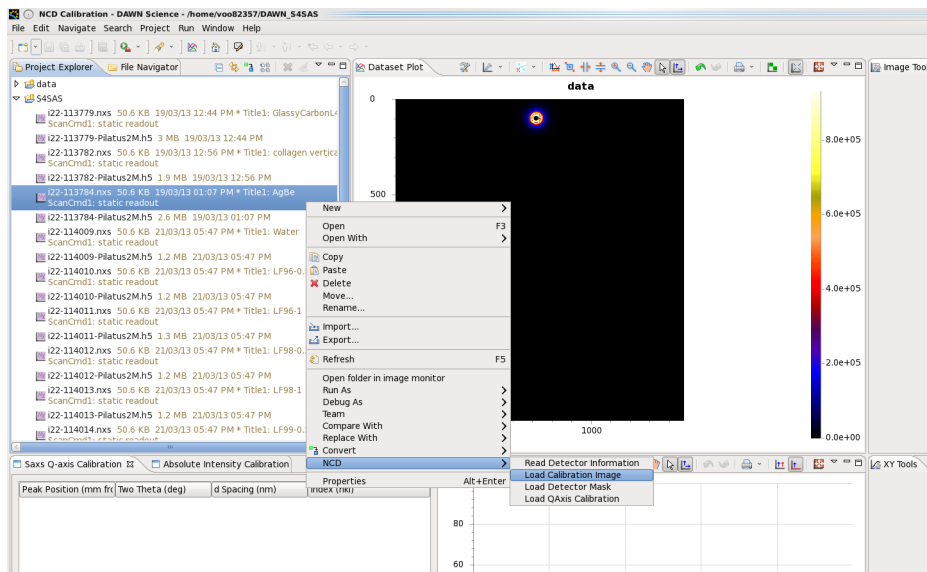


8. Navigate through S4SAS project and select one of the .nxs files. Right-click on the file to open a pop-up menu and select NCD -> Read Detector Information option. This should populate “NCD Detector Parameters” view with available detector options.

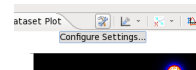


9. In “NCD Detector Parameters” view check SAXS checkbox and select It from “Normalisation Dataset” drop-down menu.

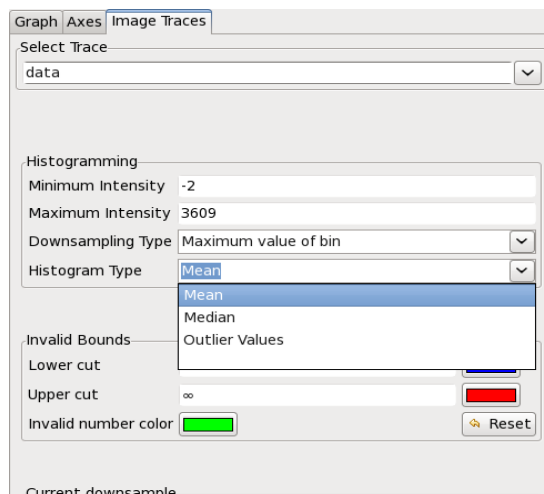
10. Select **i22-113784.nxs** file in “Project Explorer” with silver behenate calibration data and from right-click pop-up menu select NCD -> Load Calibration Image.



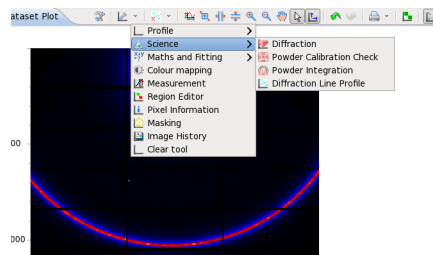
11. For adjusting colour range open “Configure Settings...” button in the image toolbar to access “Configure Graph Settings” dialog.



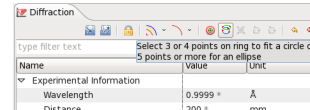
12. In the “Configure Graph Settings” dialog on “Image Traces” tab set Histogram Type to Mean.



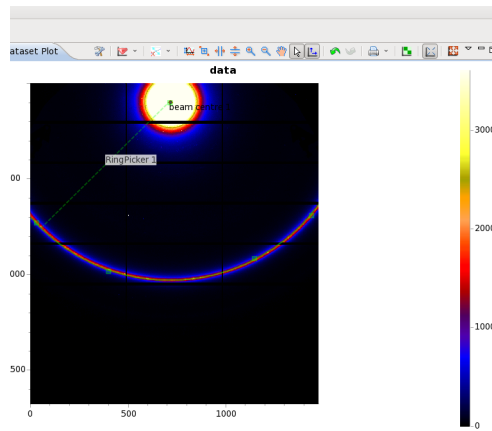
13. We will use circle fitting in Diffraction tool to find beam centre. From “Image Tools” drop-down menu in the image toolbar select Science -> Diffraction menu.



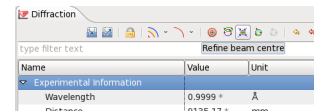
14. In the Diffraction tool toolbar select point selection button for selecting pixels for circle fitting.



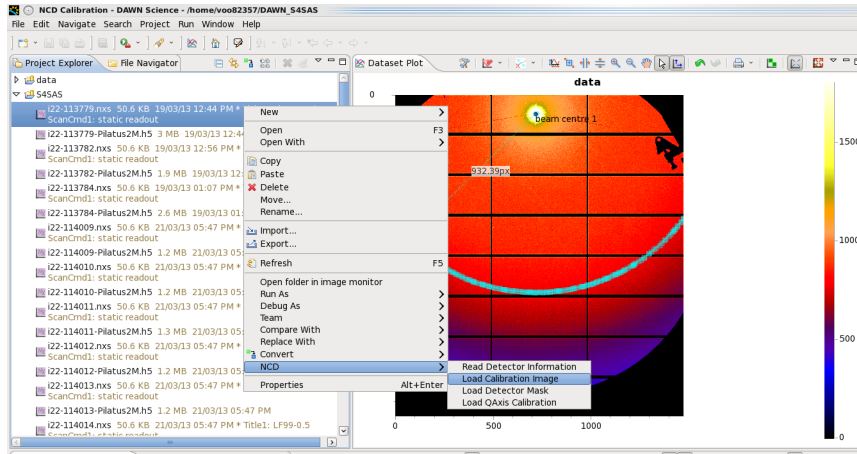
15. Make three single-clicks to pick three positions on the ring and double-click to pick the final position and run circle fitting.



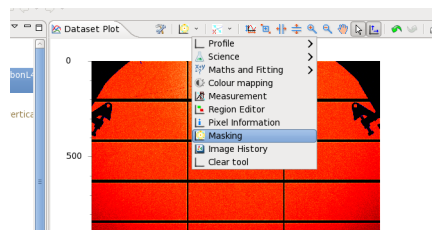
16. In the Diffraction tool toolbar click on “Refine beam centre” button to refine original circle fitting result.



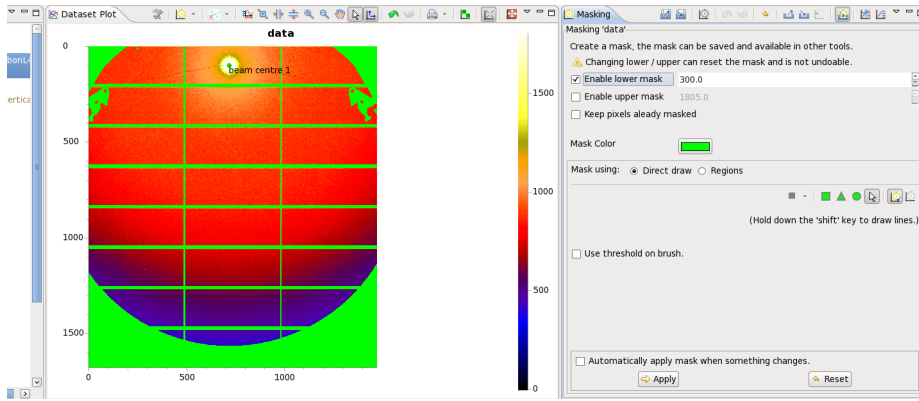
17. We will use glassy carbon dataset to quickly mask shadows on the image. Select **i22-113779.nxs** file and select NCD -> Load Calibration Image from right-click pop-up menu.



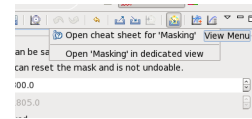
18. From the image plot toolbar select “Masking” tool.



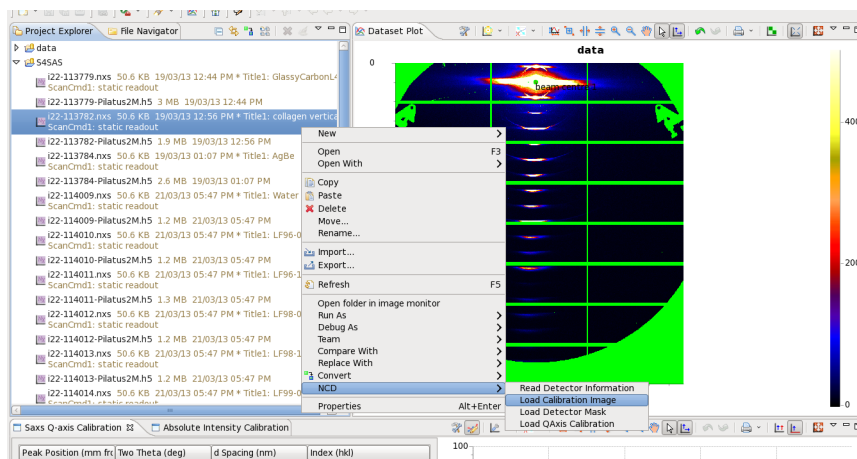
19. Select “Enable lower mask” checkbox and set value to 300.



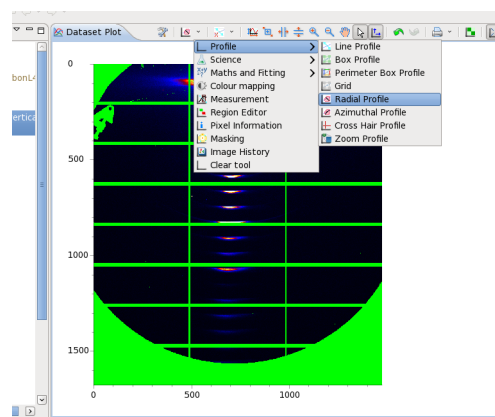
20. To preserve mask plot over different images, move “Masking” page into a separate view selecting “open “Masking” in dedicated view” option from top-right drop-down menu.



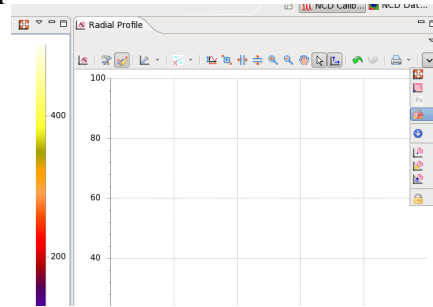
21. We will use a rat-tail collagen dataset to calibrate the data. In “Project Explorer” view select **i22-113782.nxs** file and use NCD -> Load Calibration Mask Image option from pop-up menu to load the image.



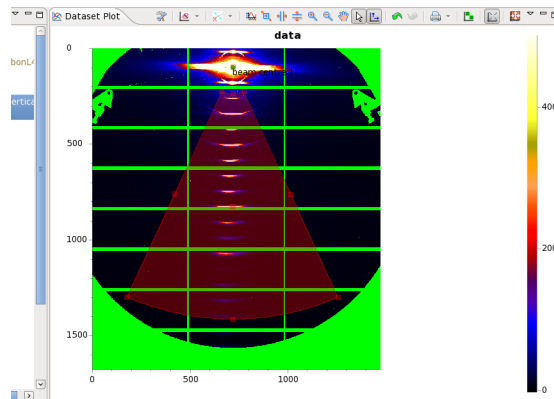
22. We need to set up sector region for integrating 2D image data. Select “Radial Profile” tool from image toolbar tools list.



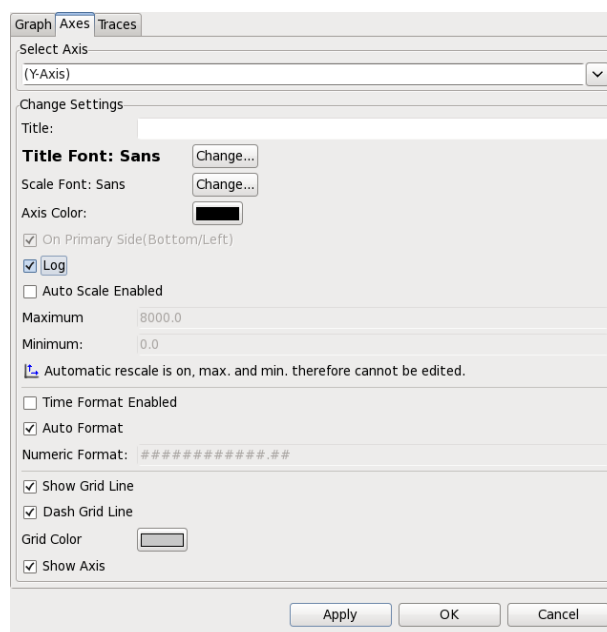
23. In the “Radial Profile” toolbar select “Lock to Metadata” button to get origin of the sector fixed to the beam centre position.



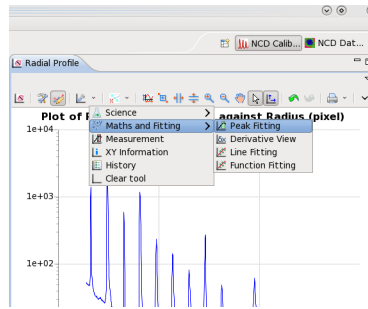
24. Define sector by clicking on the image. First click defines the sector origin (it's automatically set to beam centre as we have set the lock in the previous stage). Second click defines left corner on an inner arc of the sector and the last click sets the right corner on an outer arc. Sector size can be adjusted by dragging highlighted vertices on the perimeter of the sector.



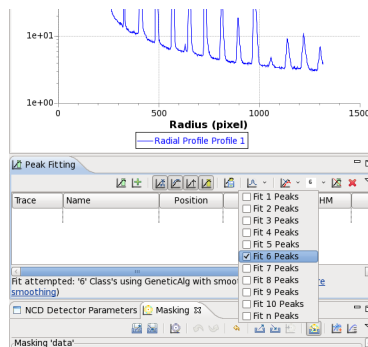
25. After sector region is set, integrated scattering profile plot will appear in the “Radial Profile” tool view. To get a better view of the integrated data we can switch Y-axis to log scale. In “Configure Graph Settings” dialog on Axes tab select (Y-axis) from Select Axis drop-down menu and check Log checkbox.



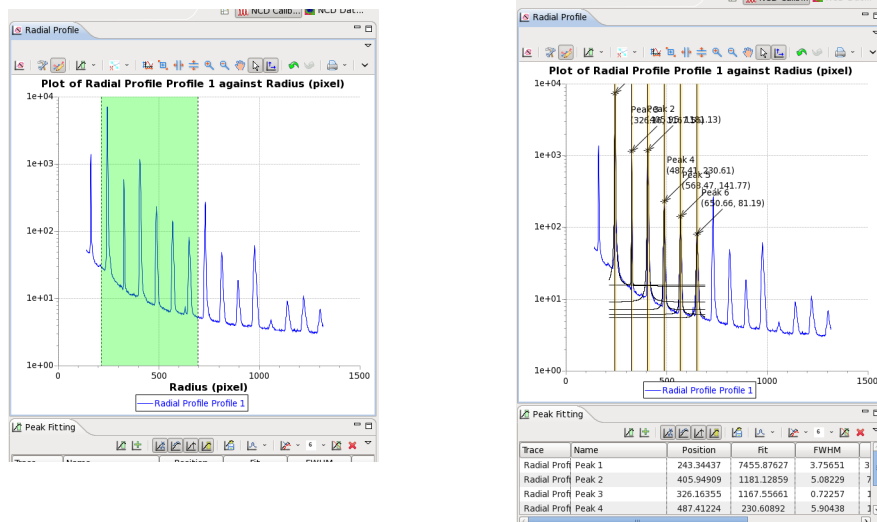
26. From tools menu select “Peak Fitting” tool.



27. In the “Peak Fitting” view toolbar select “Fit 6 Peaks” from the number of peaks drop-down menu.

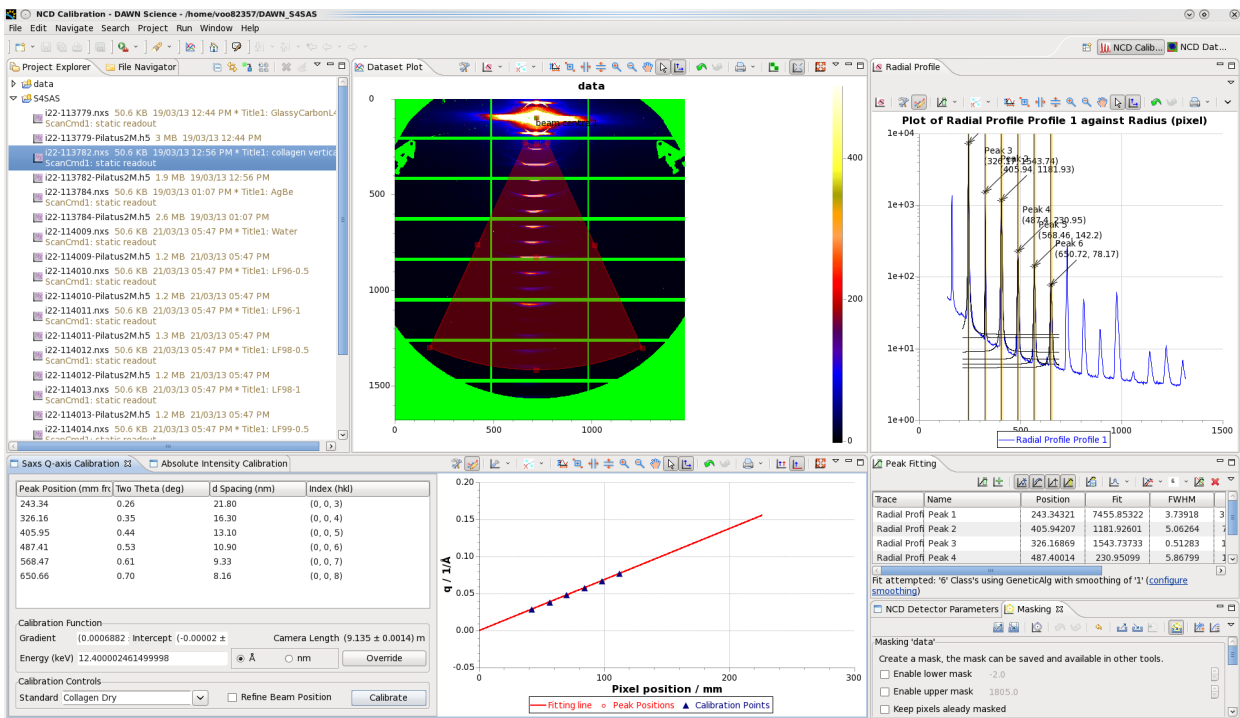


28. On the “Radial Profile” plot click and drag mouse over an area containing 6 peaks.

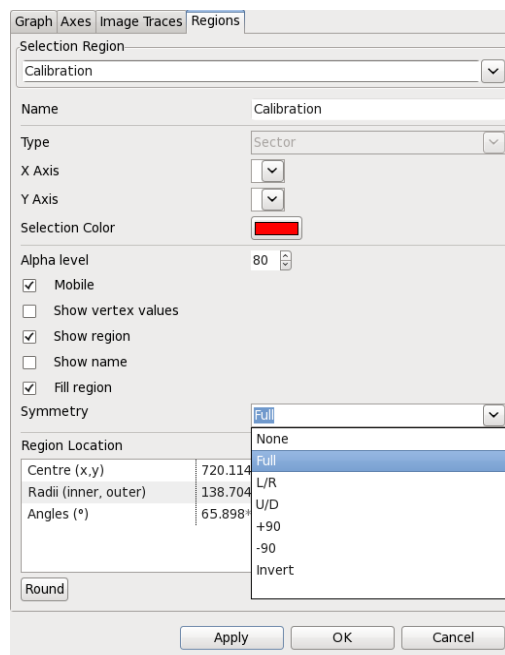


29. Peak fitting results should appear when mouse is released.

30. In “SAXS Q-axis Calibration” view select “Collagen Dry” in the Standard drop-down list, “Å” as unit and press “Calibrate” button to complete calibration process.



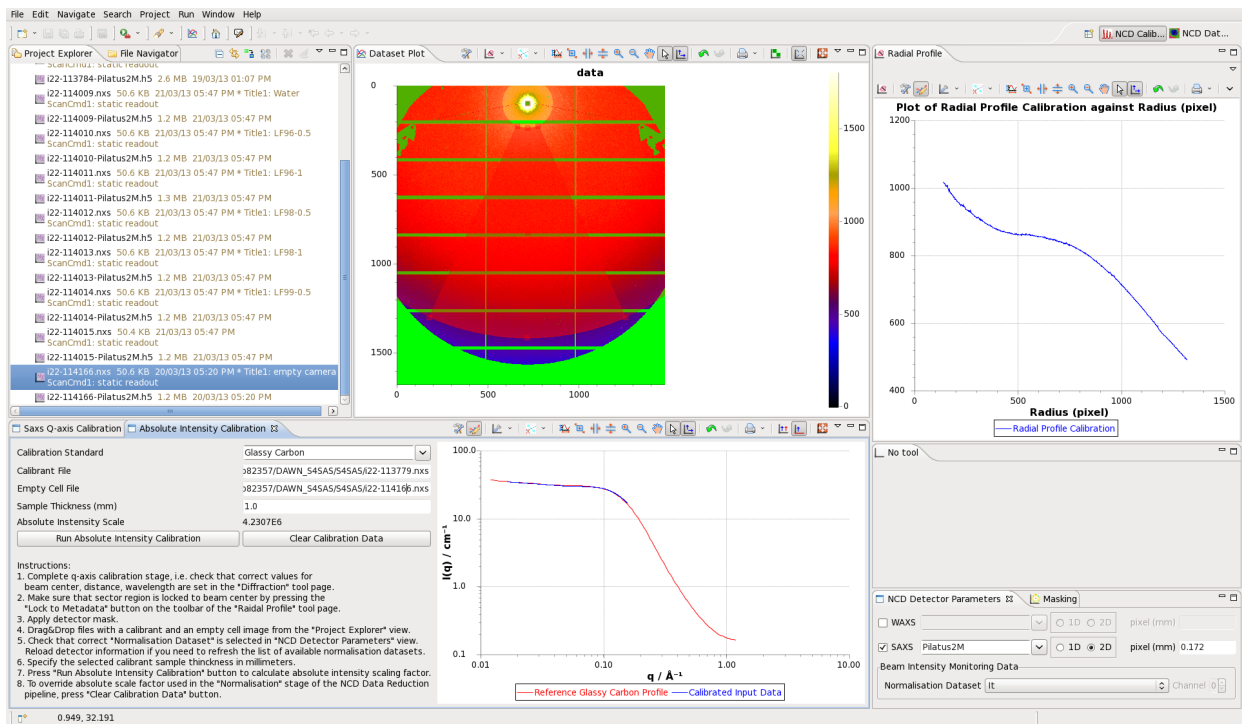
31. For further stages we will set sector region to extend full 360°. In “Configure Graph Settings” dialog on Regions page select “Full” from “Symmetry” drop-down list.



32. Click on “Absolute Intensity Calibration” tab next to “Saxs Q-axis Calibration” view to make the corresponding view visible.

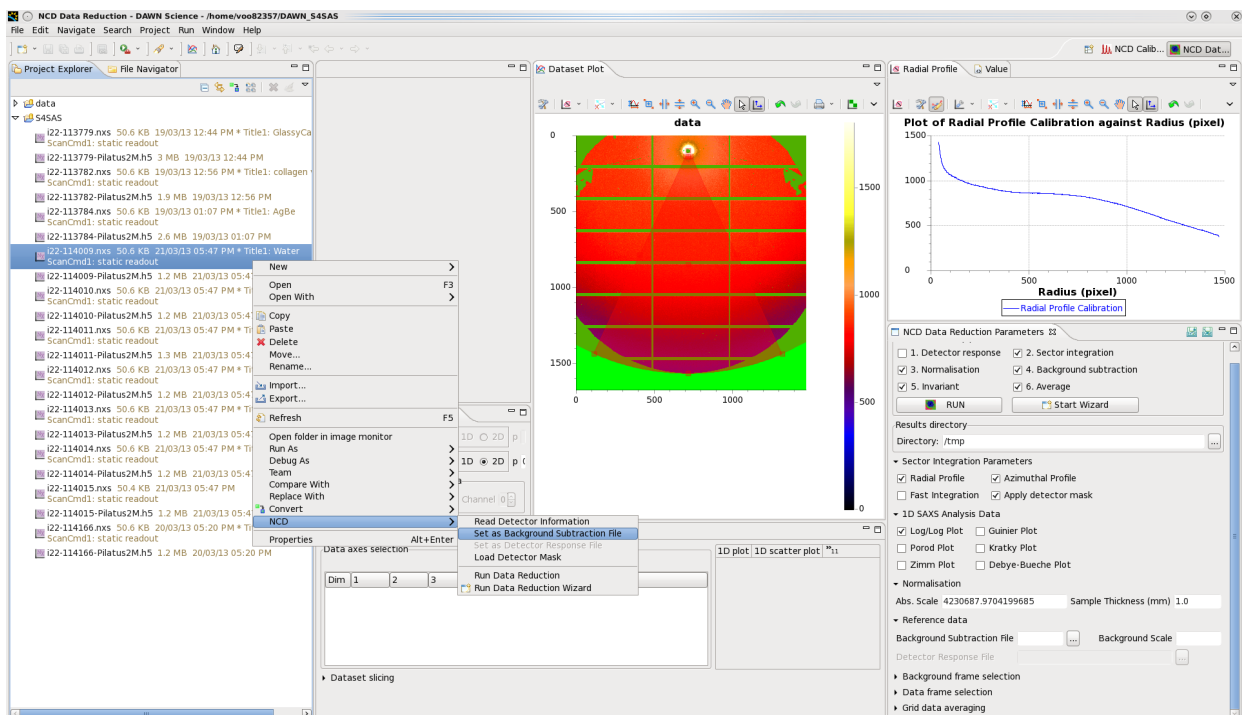
33. Drag&Drop **i22-113779.nxs** file into “Calibrant File” field and **i22-114166.nxs** into the “Empty Cell File” field.

34. Set Sample Thickness to 1.0 and press “Run Absolute Intensity Calibration” button. Scaling factor will be displayed in “Absolute Intensity Scale” field and rescaled integrated intensity profile will be overlaid on the reference glassy carbon profile in the adjacent plot.



35. Open “NCD Data Reduction” perspective by pressing the corresponding button in the top-right corner in DAWN toolbar.

36. Set data reduction parameters in the “NCD Data Reduction Parameters” view.

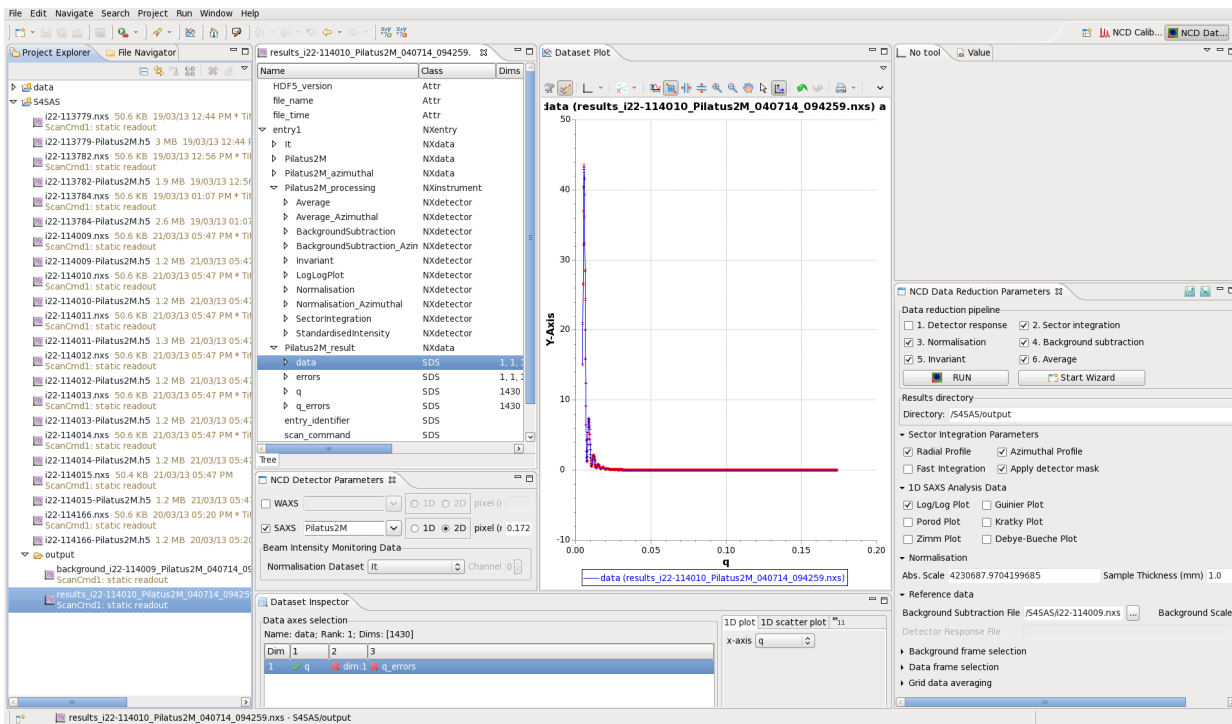


37. Select **i22-114009.nxs** file in “Project Explorer” view as set it as background file by selecting NCD -> Set as Background Subtraction File option from a right-click pop-up menu (alternatively, drag&drop this file into “Background Subtraction File” field in “NCD Data Reduction Parameters” view).

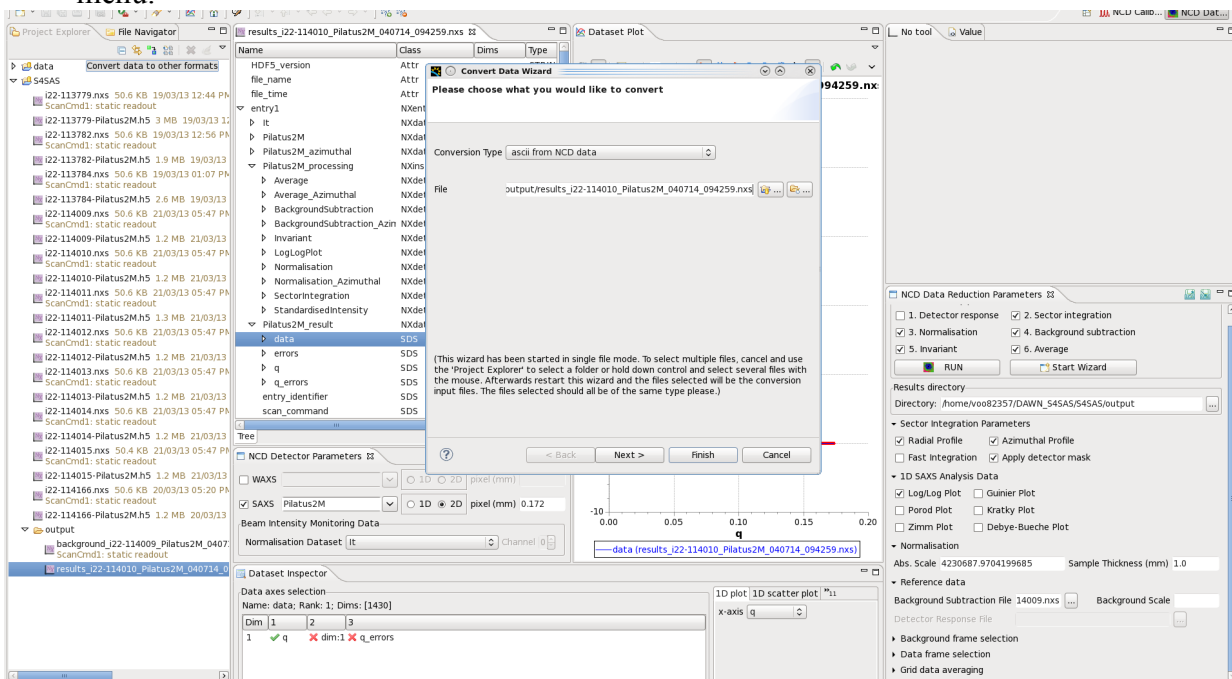
38. To specify location where reduced data files will be written, drag&drop output directory within S4SAS project into “Directory” field in “NCD Data Reduction Parameters” or use an adjacent “...” button to pick the desired directory in the File Open dialog.

39. Select files from **i22-114010.nxs** to **i22-114015.nxs** in “Project Explorer” (hold SHIFT key to select the full file range or CTRL to select individual files) and press “RUN” button .

40. Select output directory in S4SAS project and press “F5” to refresh the contents. Double-click on one of the results .nxs files to view data hierarchy. Double-click on /entry1/Pilatus2M_result/data node to plot the reduced 1D profile. Results from the intermediate processing stages are available in /entry1/Pilatus2M_processing node.



41. To export data from the results files into other formats press “Convert data” button in the “Project Explorer” toolbar or use Convert -> Convert Wizard... option from right-click menu.



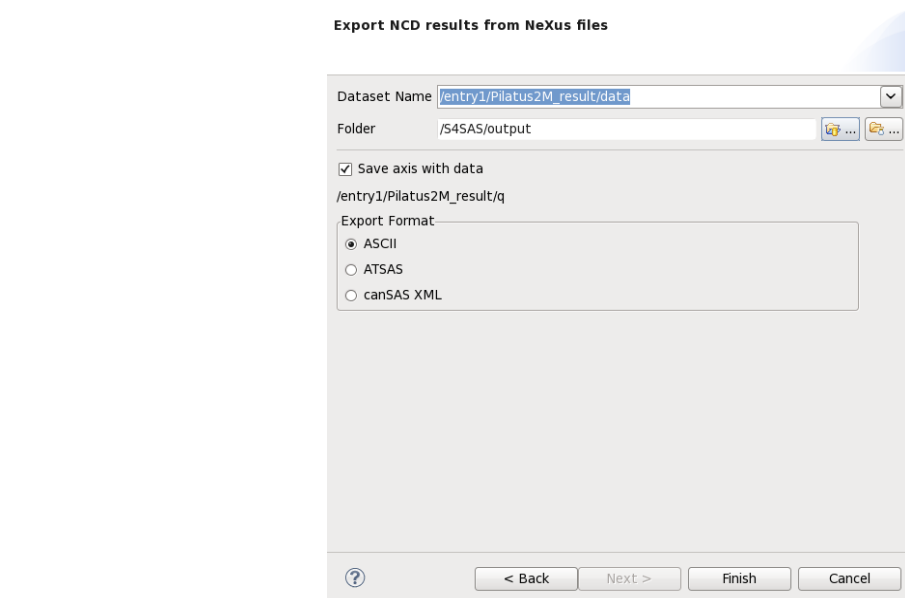
42. Select “ascii from NCD data” in conversion type drop-down menu and press “Next >”.

43. Select required dataset of interest (e.g. /entry1/Pilatus2M_result/data) in “Dataset Name” drop-down list. Output directory can be selected in “Folder” field. Following formats are available:

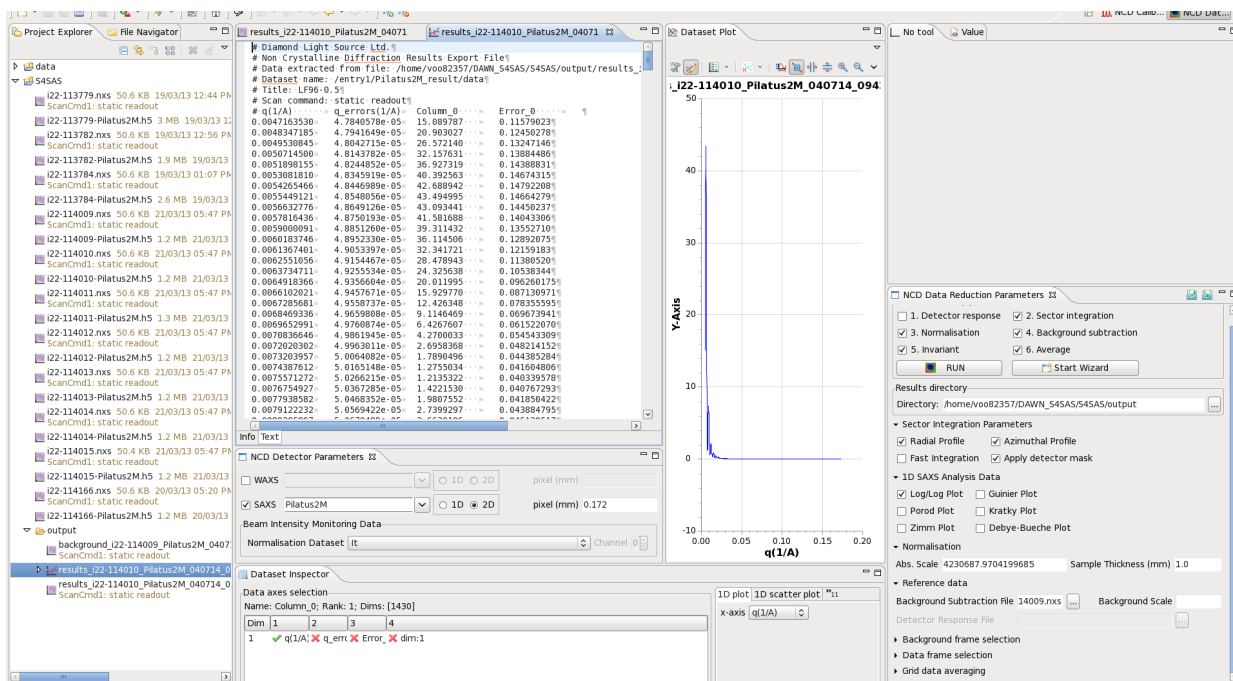
ASCII – multicolumn text file.

ATSAS – text file compatible with EMBL ATSAS software for solution scattering.

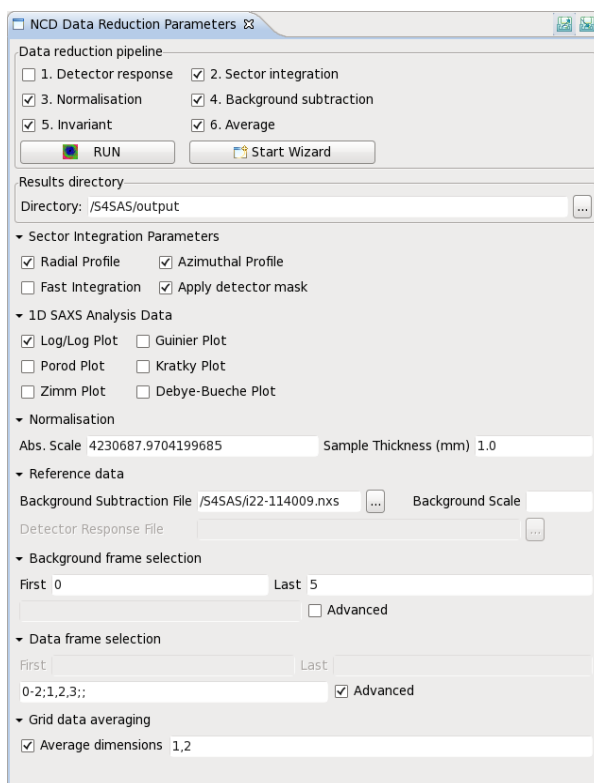
canSAS XML – XML files for SasView ver. > = 2.2.1



44. Press “Finish” to export the data. You can browse exported files by double-clicking on the in “Project Explorer” view.



45. (Illustration) Options for processing and averaging subset of data are available in “NCD Data Reduction Parameters” view. Details, together with guides for other functionality in DAWN, are available in Help -> Cheat Sheets... pages.



46. For reporting problems or providing general feedback regarding DAWN functionality, please use the feedback form available from Help -> Leave Feedback menu of from <http://www.dawnsi.org/> website.

The screenshot shows the 'Feedback' form with the following fields and options:

- Send Feedback to:** Radio buttons for 'DAWN developers' (selected) and 'DAWN mailing list'.
- Your email address for Feedback:** A text input field.
- Summary:** A text input field.
- Comment:** A large text area for detailed feedback.
- Attached Files:** A list of files with an 'Attach Files' button below it.
- Buttons:** 'Attach Files' and 'Send Feedback' buttons at the bottom.