



QtSAS v. 2023-01-24

QtSAS | Preferences | QtSAS | Image+Project :: Image Format

- ✓ [1.1] PDF-Image format is added; graphs are saved like a image

QtSAS | Print Preview | [Scale Layers to paper size]

- ✓ [1.2] scaling and positioning is improved

Fit.Curve(s) | Pasting to the active graph of the table of datasets and parameters

- ✓ [1.3] the table of datasets and parameters contains now “paste” button in the corner header cell



DAN | Options

- ✓ [2.1] SAS-detector could be ROTATED around the sample position. Detector rotation angles around the sample position (within horizontal and vertical planes) are integrated into data analysis algorithms.

DAN | Rawdata Tools | Info Extractor

- ✓ [2.2] selection of the subfolder is implemented

DAN | Rawdata Tools | Image(s) to Info-Matrix

- ✓ [2.3] added a new button to add block of matrixes from an active table

DAN | Data Processing | Options :: [1D] | I[Q] :: Radial Averaging :: Method

- ✓ [2.4] linear merging option is implemented; progressive merging is optimized [during a single detector image radial averaging]

DAN | Data Processing | Options :: Script Table

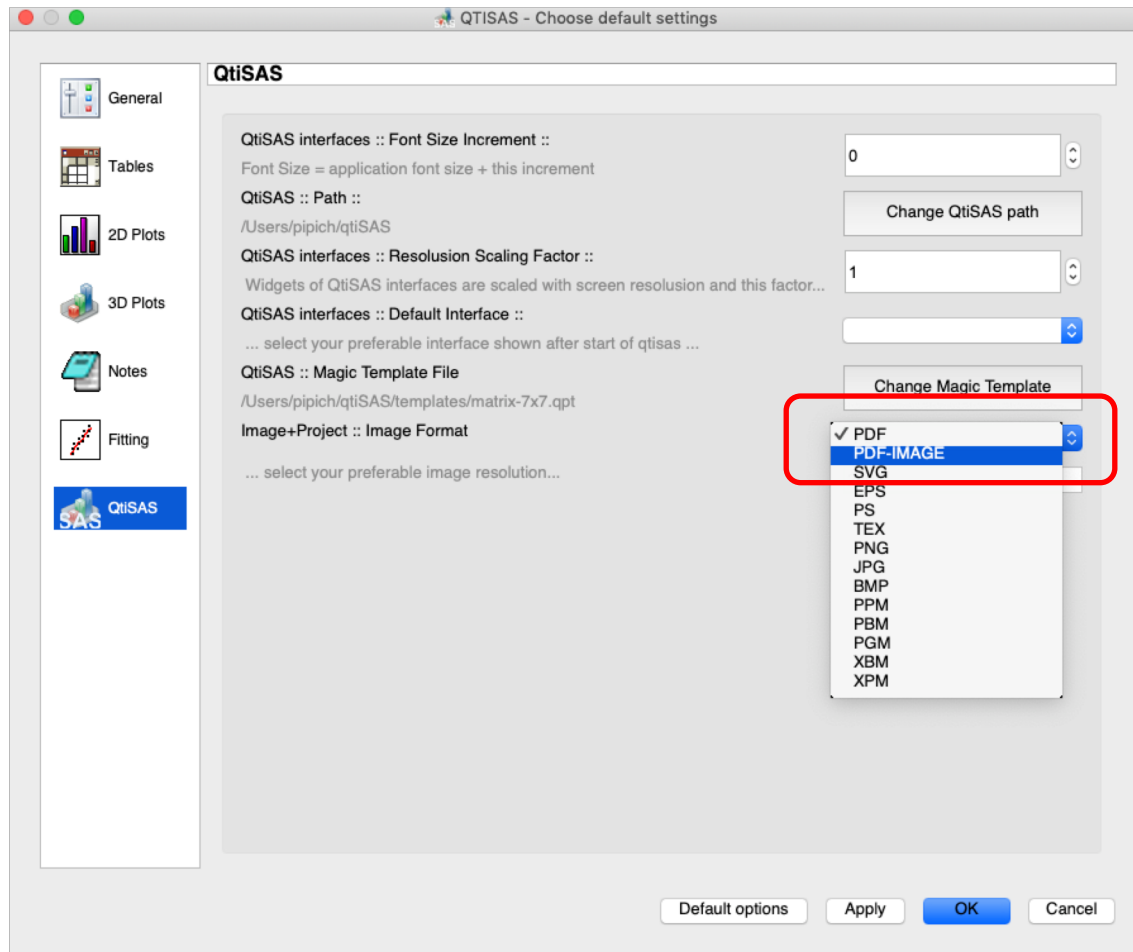
- ✓ [2.5] check-boxes are re-ordered to several groups;
- ✓ [2.6] implemented buttons for the absolute factor calculation within the current script table (in the case of the direct beam absolute calibration) and transmission calculation

DAN | Merge | Merge by Re-Binning

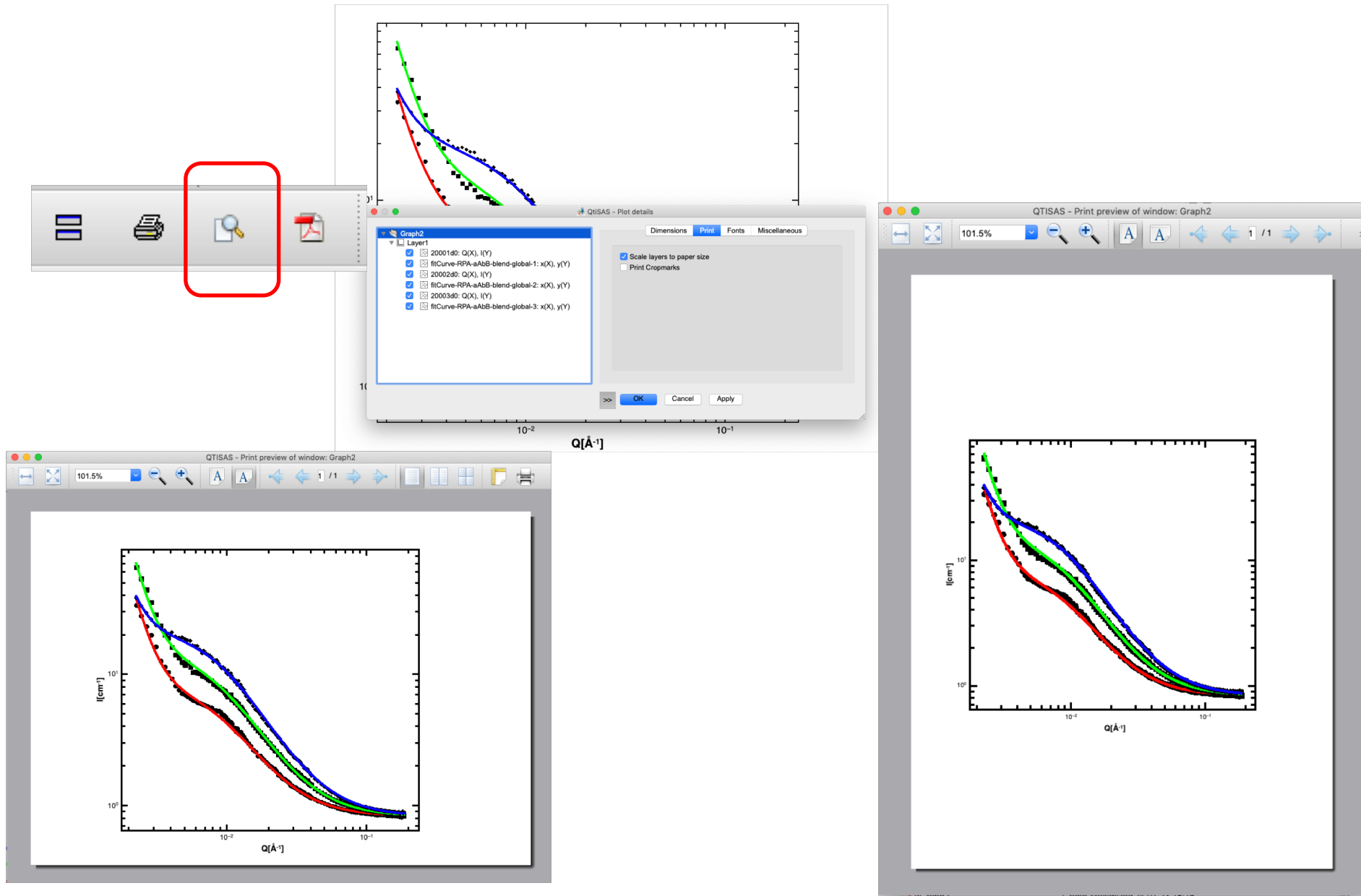
- ✓ [2.7] second way of merging implemented in the DAN-SANS. Re-binning with pre-defined steps in the q-space (linear or logarithmic) is possible. This is specially important by merging of the TOF channels.

QtiSAS | Preferences | QtiSAS | Image+Project :: Image Format

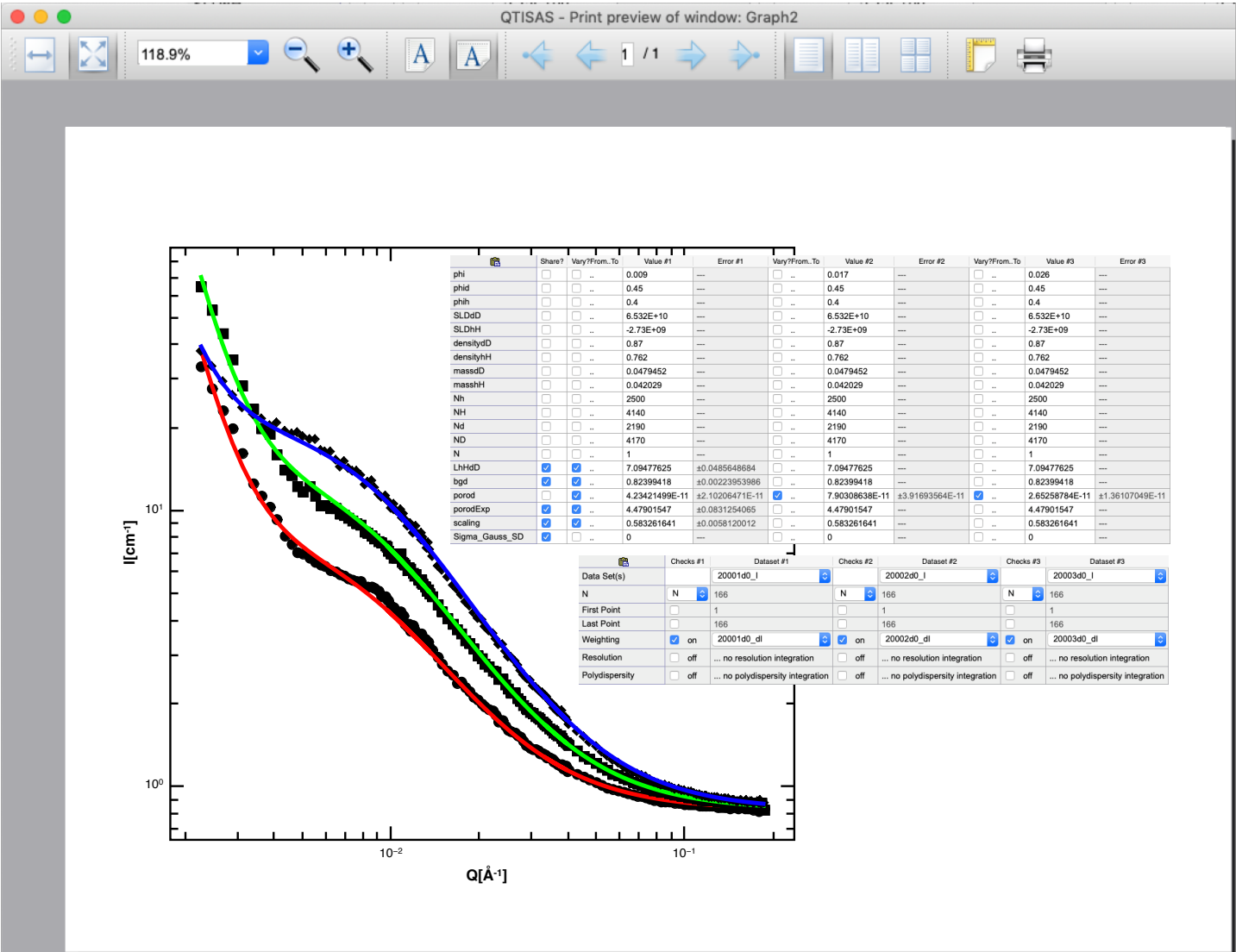
[1.1] PDF-Image format is added; graphs are saved like a image



[1.2] scaling and positioning is improved

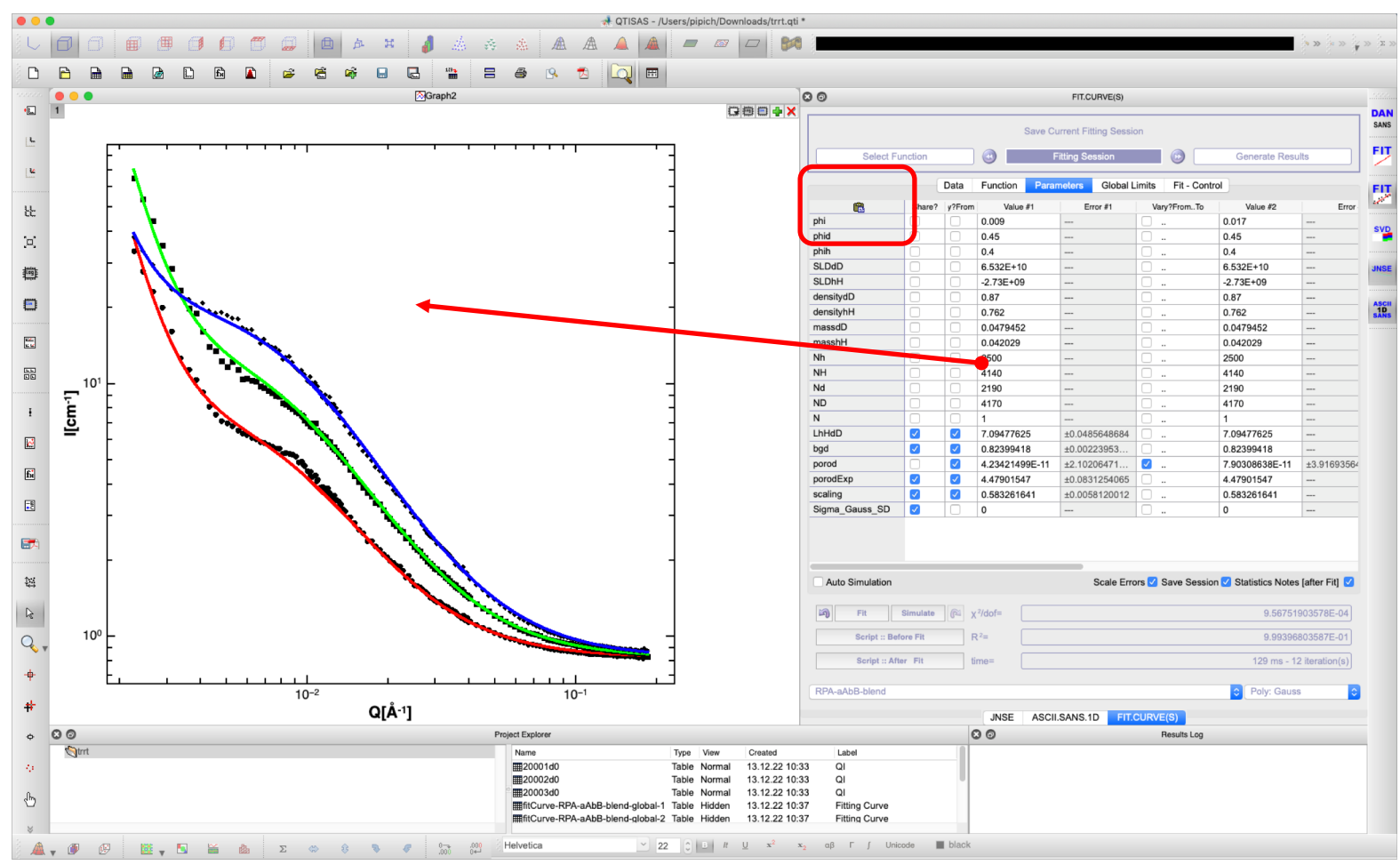


[1.2] scaling and positioning is improved



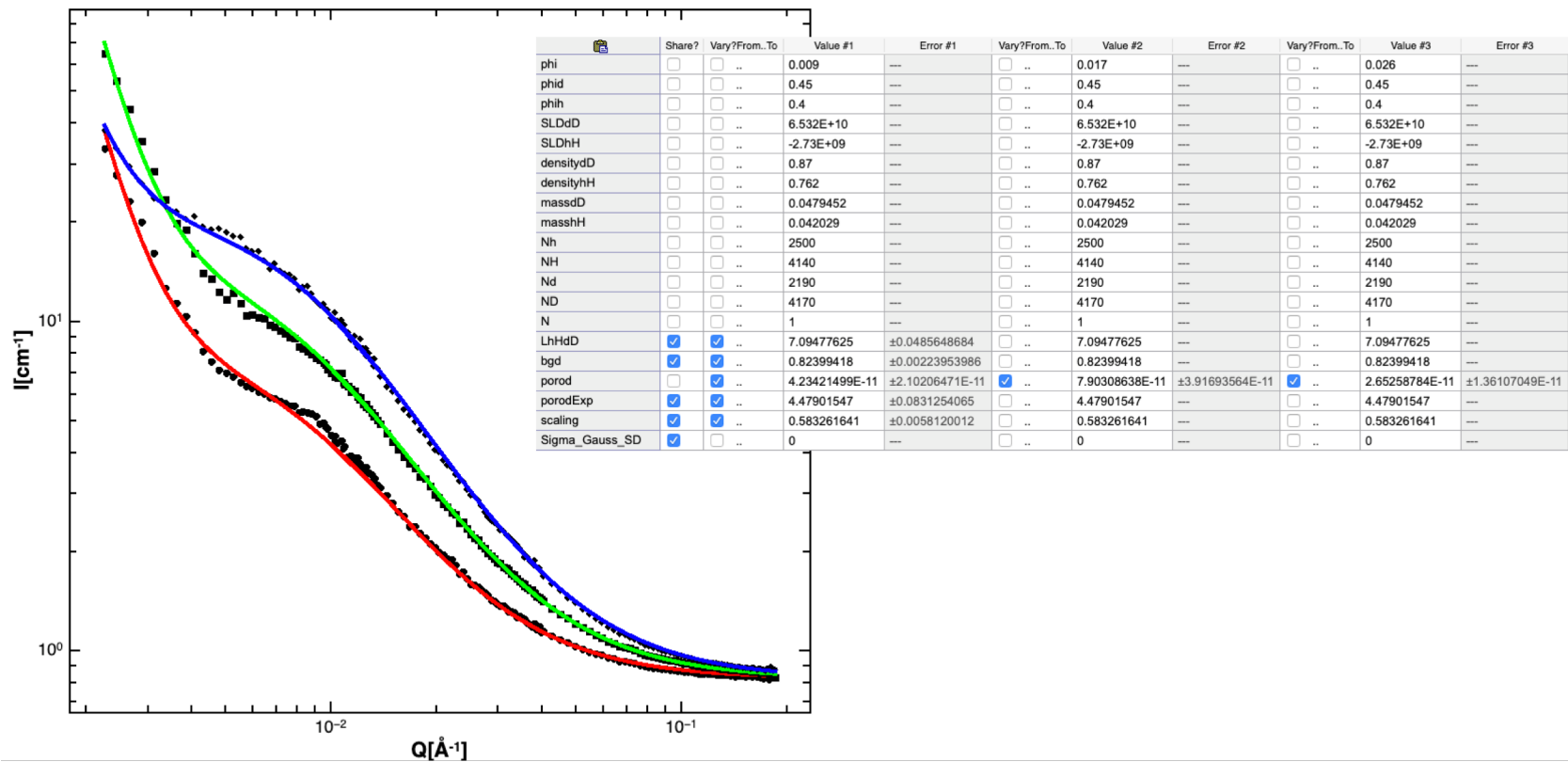
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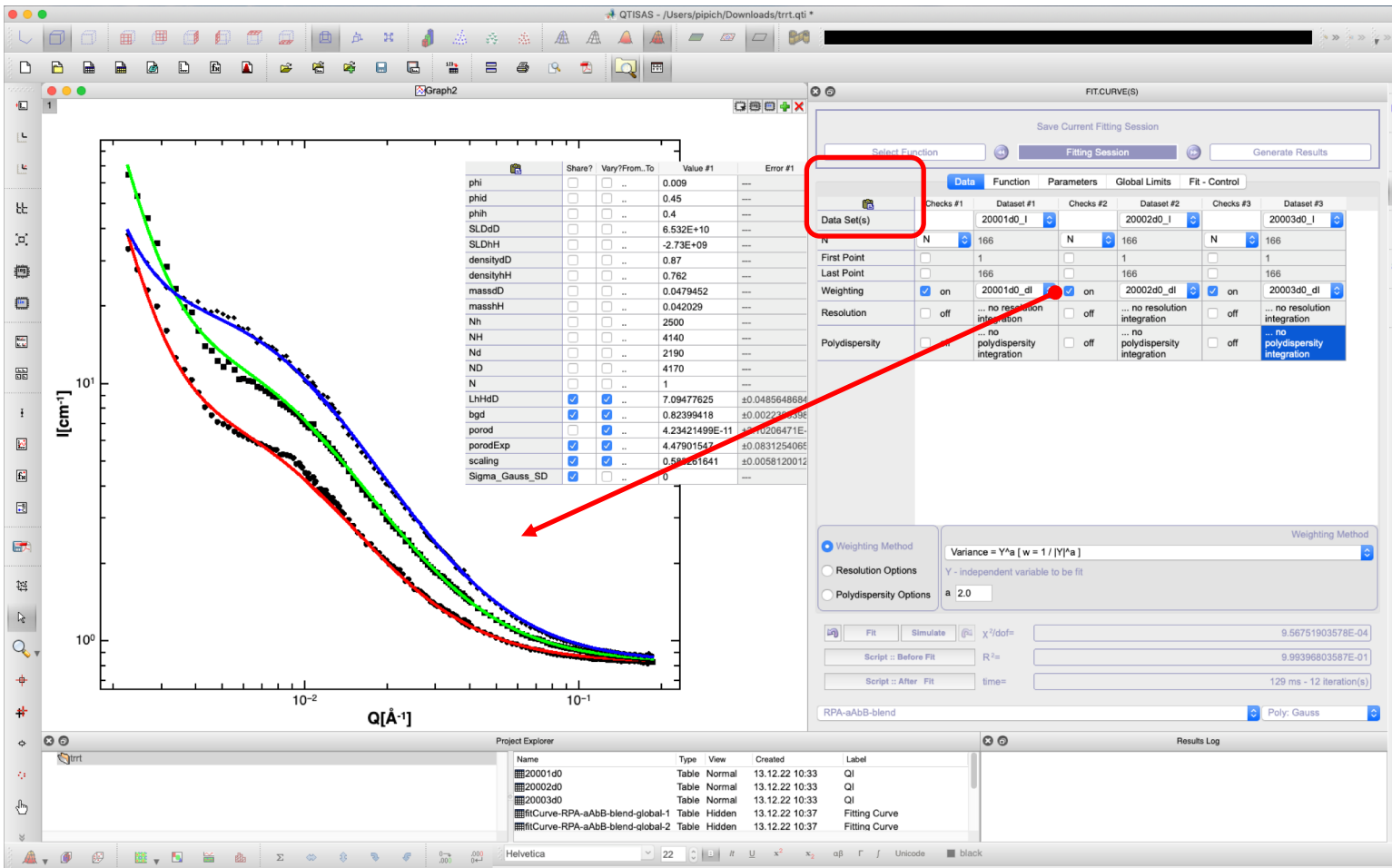
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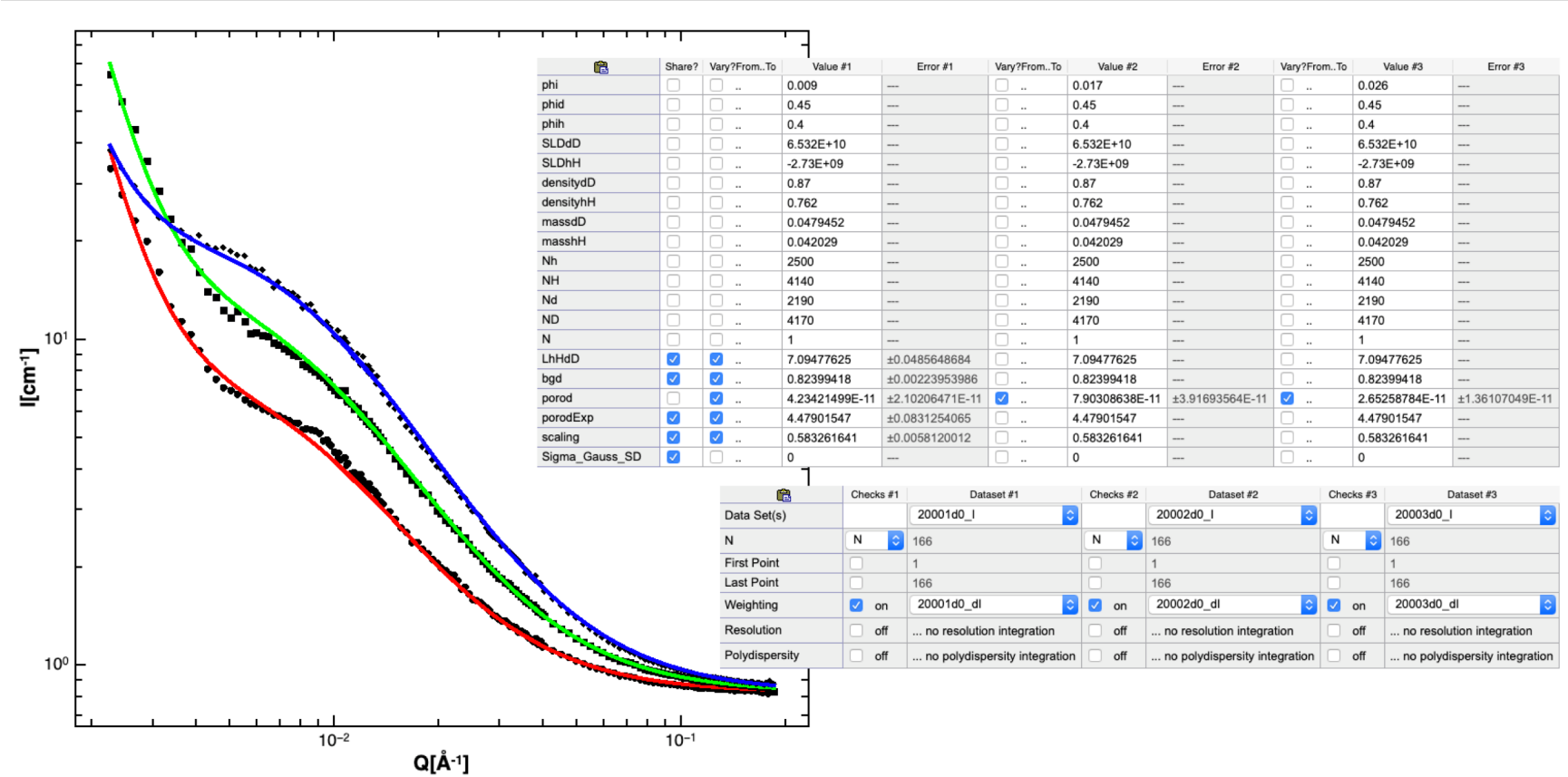
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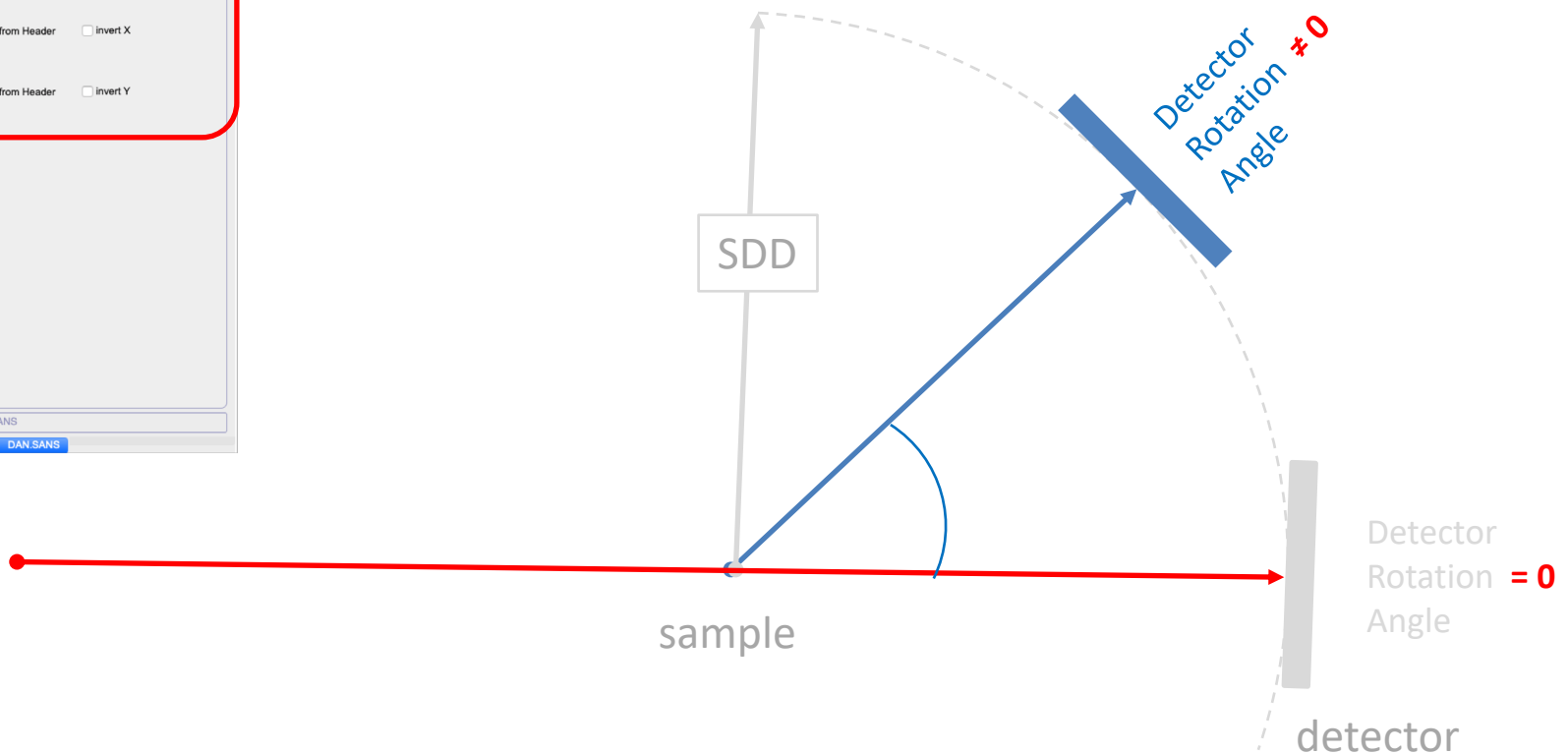
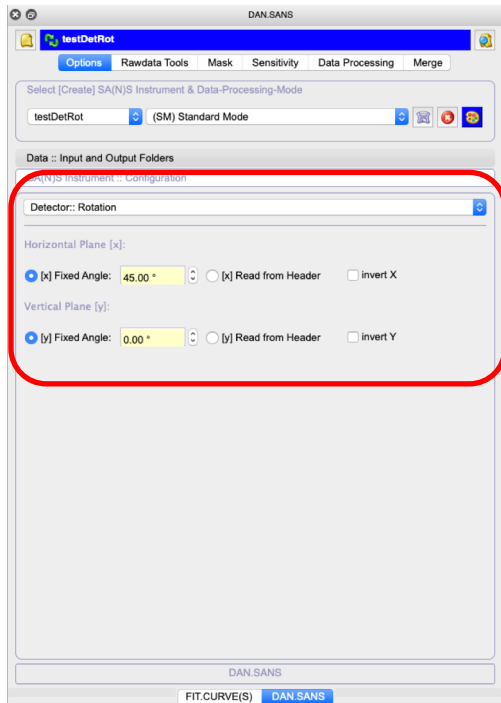
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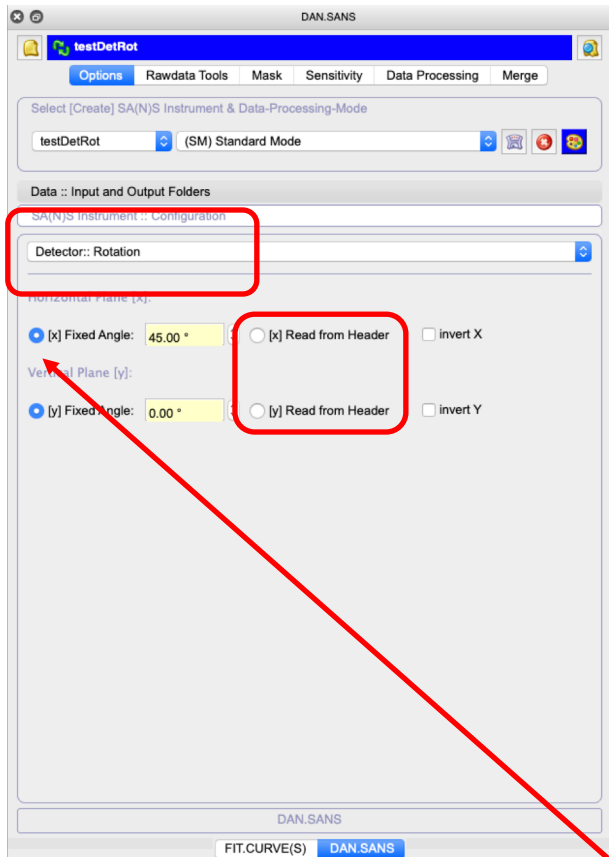
DAN | Options

[2.1] SAS-detector could be placed off-direct-beam. Detector rotation angles around a sample position (within horizontal and vertical planes) are integrated into data analysis algorithms



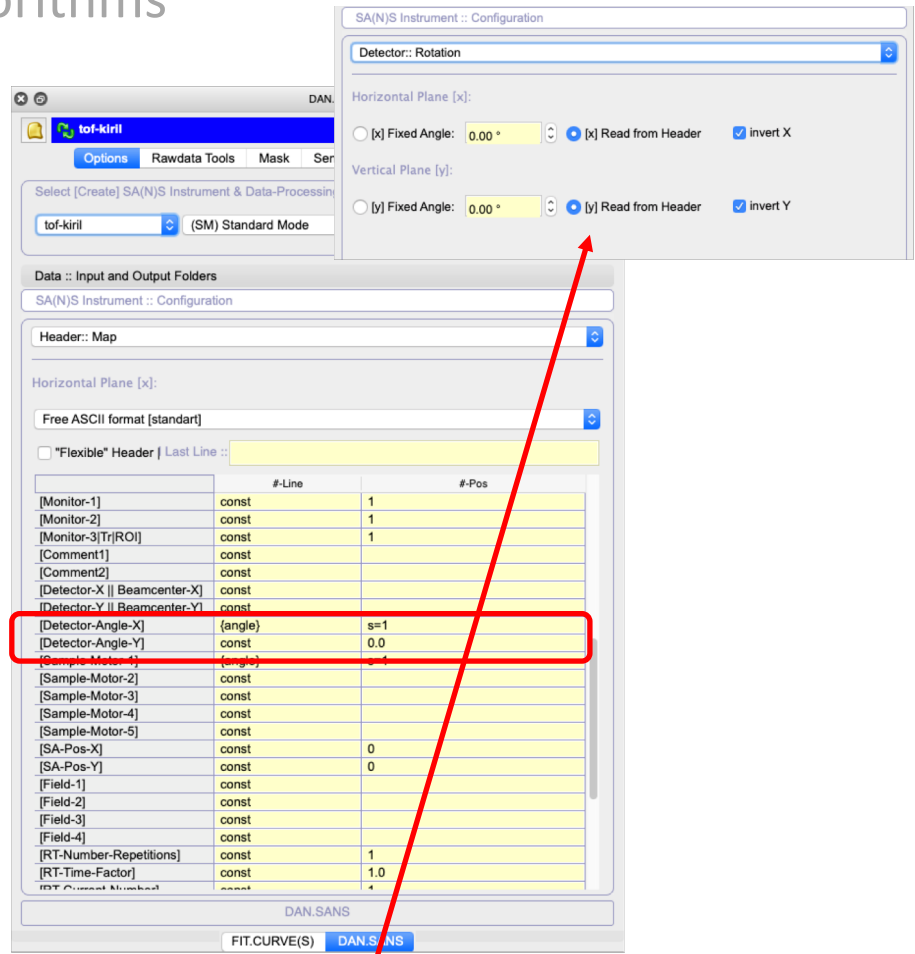
DAN | Options

[2.1] SAS-detector could be placed off-direct-beam. Detector rotation angles around a sample position (within horizontal and vertical planes) are integrated into data analysis algorithms



Detector rotation angles could be fixed

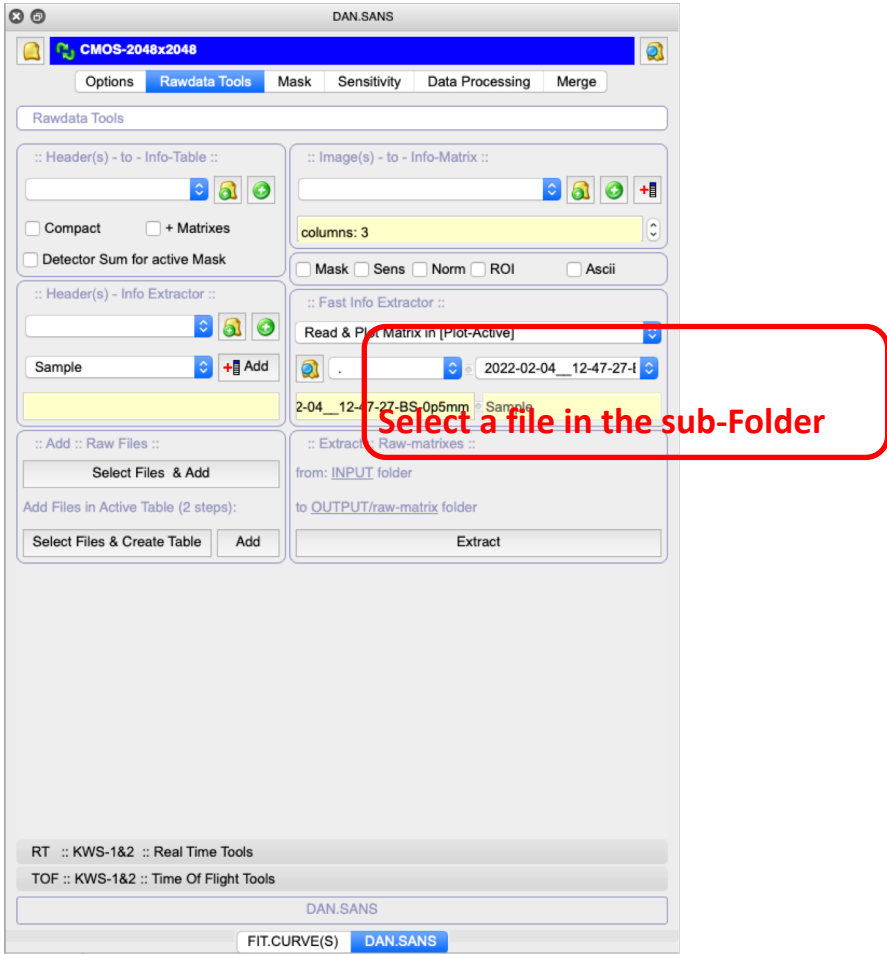
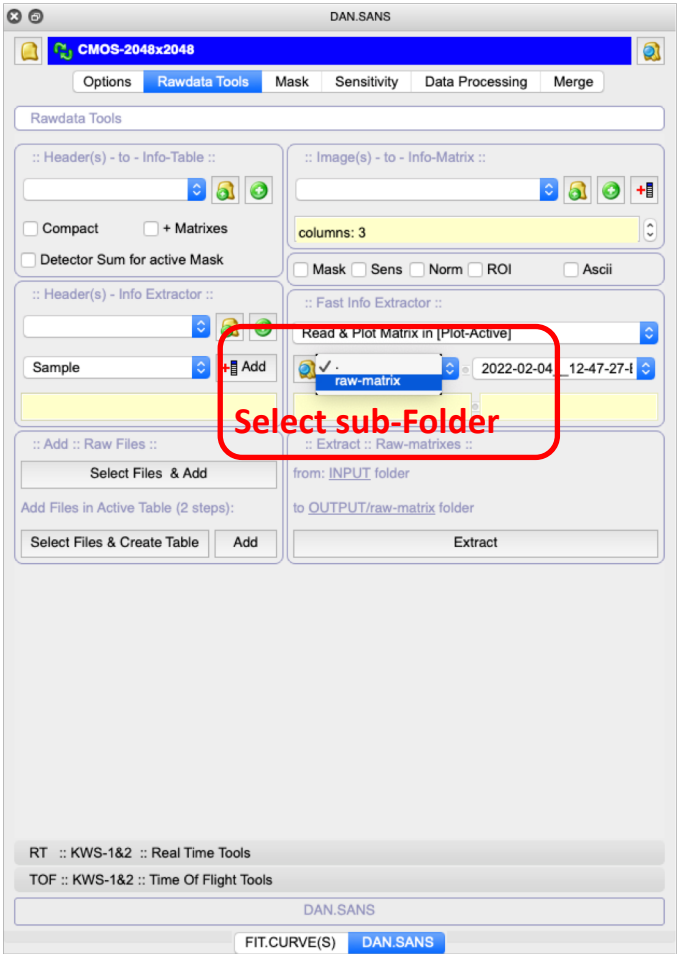
or



readable from the headers...

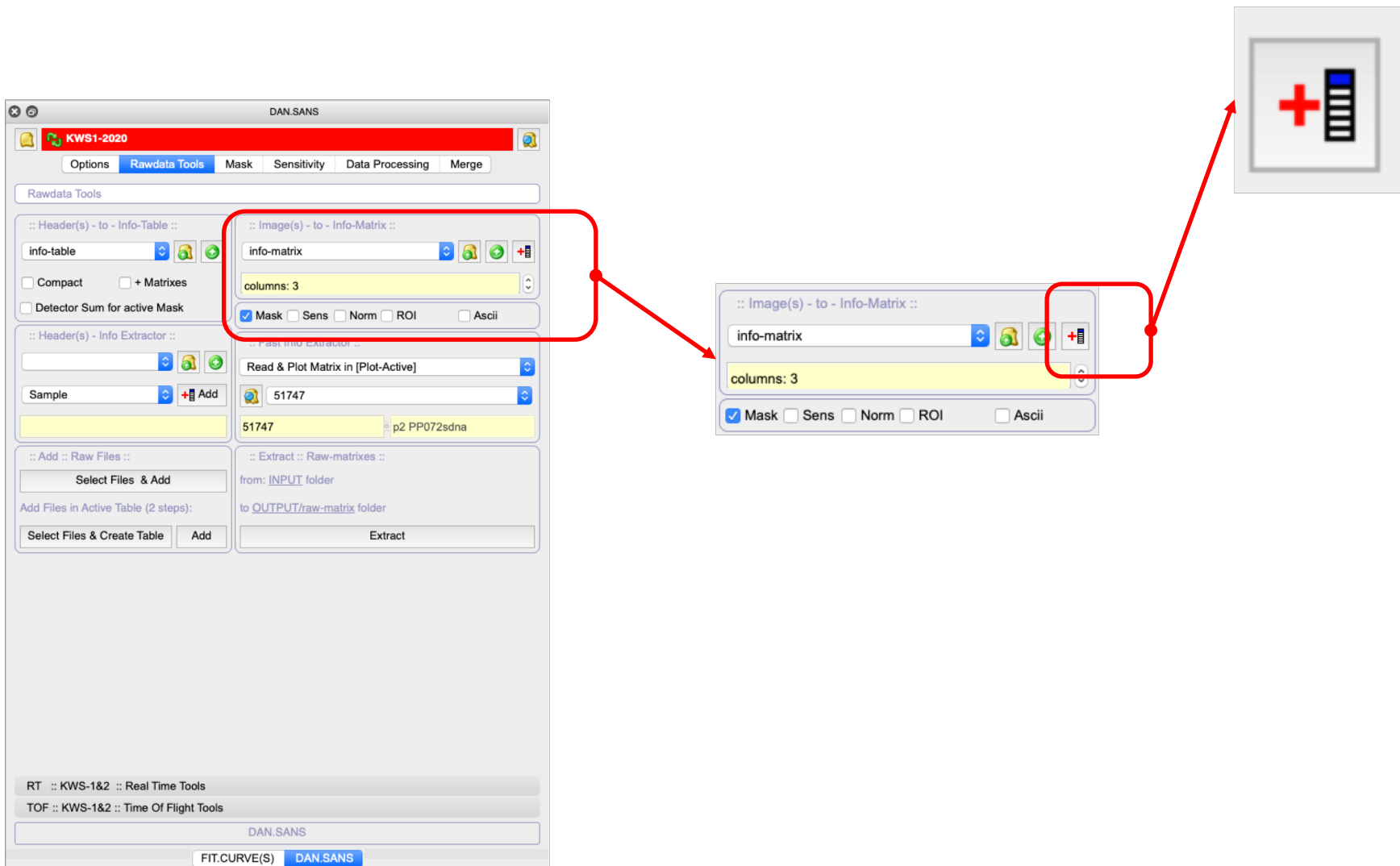
DAN | Rawdata | Info Extractor

[2.2] Selection of the subfolder is implemented

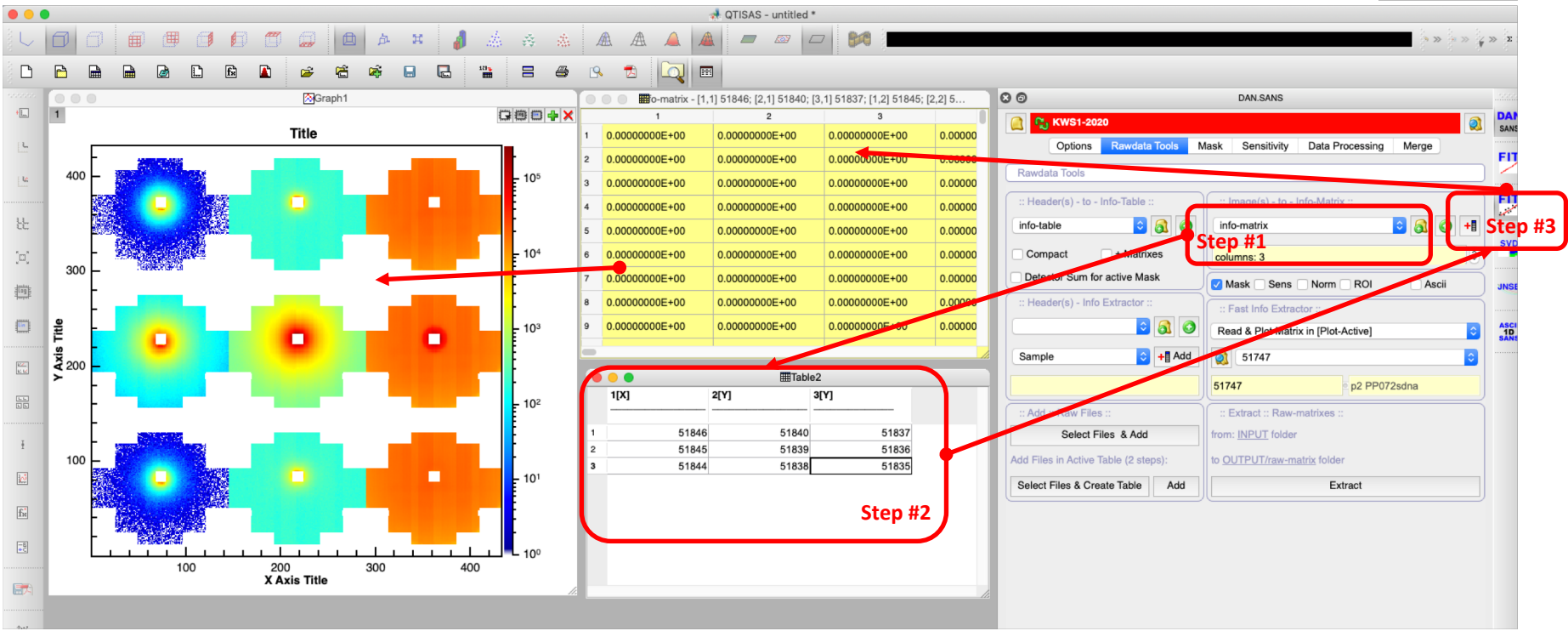


DAN | Rawdata Tools | Image(s) to Info-Matrix

[2.3] added a new button to add block of matrixes from an active table

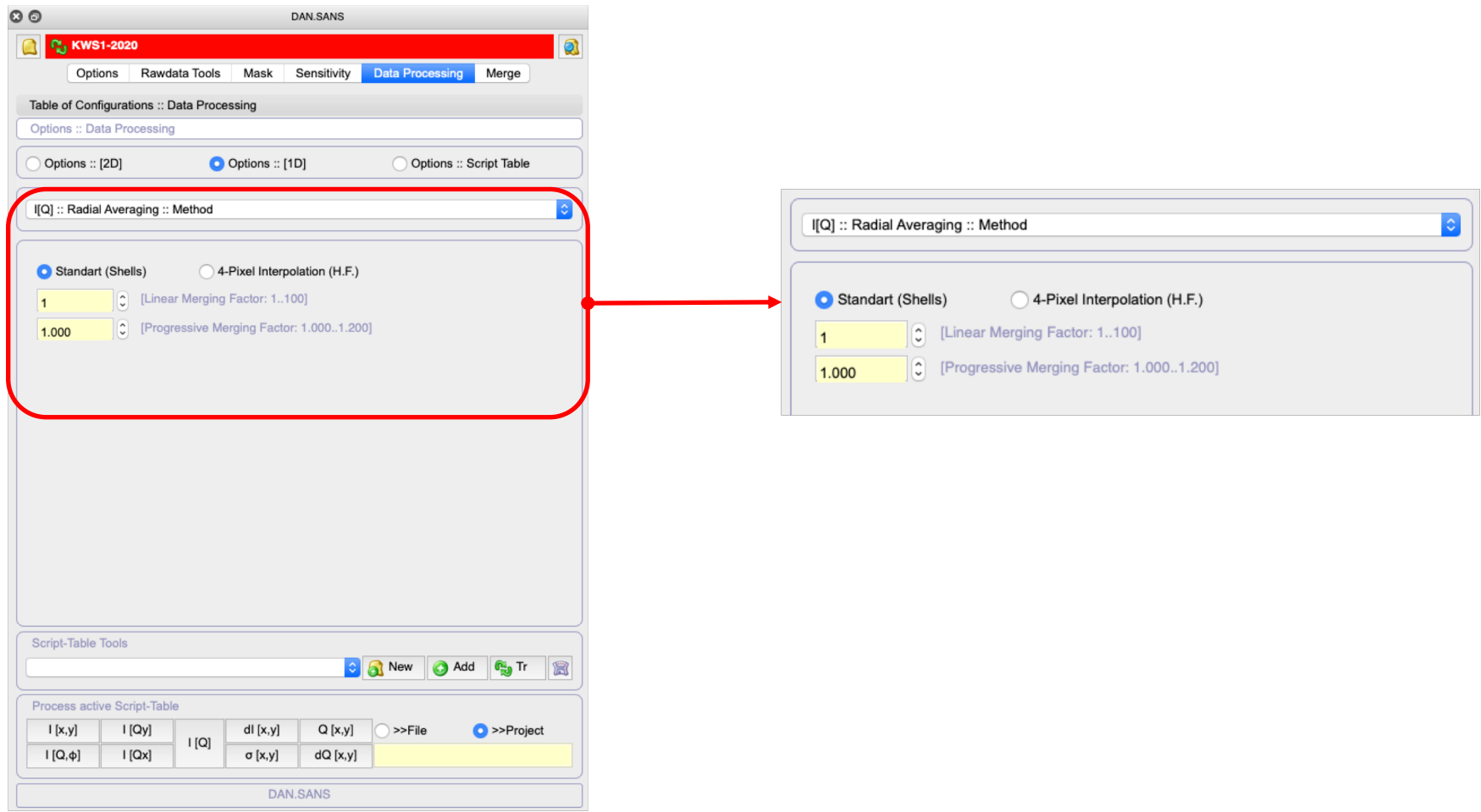


[2.3] added a new button to add block of matrixes from an active table



- #1 creation of the empty matrix with defined number of column ["info-matrix"]
- #2 manually filling of the table with run-numbers
- #3 pushing of the NEW button
- #4 plotting of the ["info-matrix"]

DAN | Data Processing | Options :: [1D] | I[Q] :: Radial Averaging :: Method
[2.4] linear merging option is implemented; progressive merging is optimized
[during a single detector image radial averaging]



DAN | Data Processing | Options :: Script Table

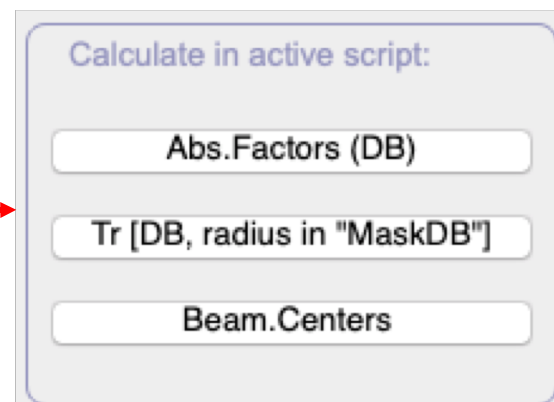
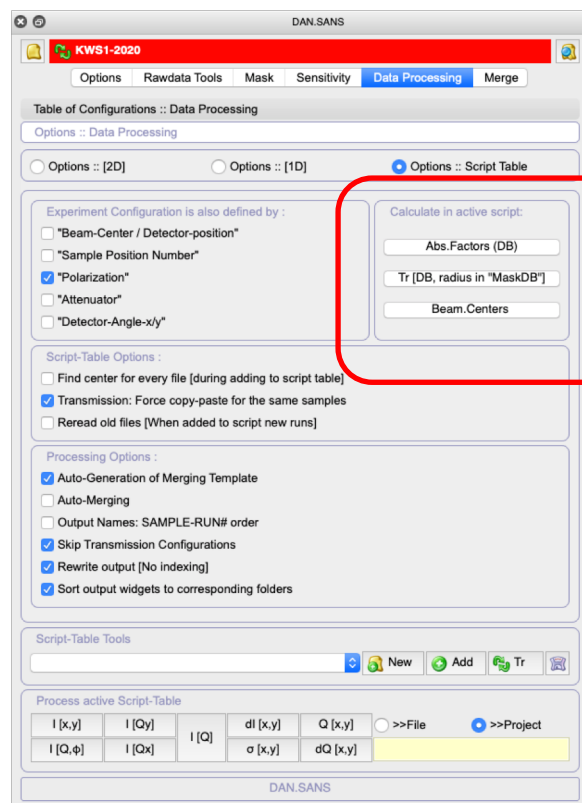
[2.5] check-boxes are re-ordered to several groups;

The screenshot shows the 'DAN.SANS' application window with the 'Data Processing' tab selected. The 'Options :: Script Table' radio button is active. The interface is organized into several sections:

- Table of Configurations :: Data Processing**
 - Options :: Data Processing
 - Options :: [2D] (inactive), Options :: [1D] (inactive), Options :: Script Table (active)
- Experiment Configuration is also defined by :**
 - ☐ "Beam-Center / Detector-position"
 - ☐ "Sample Position Number"
 - ☒ "Polarization"
 - ☐ "Attenuator"
 - ☐ "Detector-Angle-x/y"
- Calculate in active script:**
 - Abs.Factors (DB)
 - Tr [DB, radius in "MaskDB"]
 - Beam.Centers
- Script-Table Options :**
 - ☐ Find center for every file [during adding to script table]
 - ☒ Transmission: Force copy-paste for the same samples
 - ☐ Reread old files [When added to script new runs]
- Processing Options :**
 - ☒ Auto-Generation of Merging Template
 - ☐ Auto-Merging
 - ☐ Output Names: SAMPLE-RUN# order
 - ☒ Skip Transmission Configurations
 - ☒ Rewrite output [No indexing]
 - ☒ Sort output widgets to corresponding folders
- Script-Table Tools**
 - Buttons: New, Add, Tr, and a folder icon.
- Process active Script-Table**
 - Grid of variables: I [x,y], I [Qy], I [Q], dI [x,y], Q [x,y], I [Q,φ], I [Qx], σ [x,y], dQ [x,y].
 - Buttons: >>File and >>Project (active).

The bottom of the window displays 'DAN.SANS'.

[2.6] implemented buttons for the absolute factor calculation within the current script table (in the case of the direct beam absolute calibration) and transmission calculation



DAN | Merge | Merge by Re-Binning

[2.7] second way of merging implemented in the DAN-SANS. Re-binning with pre-defined steps in the q-space (linear or logarithmic) is possible. This is specially important by merging of the TOF channels.

Active Table define list of Runs to merge

The screenshot shows the 'Merge' dialog box in the DAN.SANS software. The window title is 'DAN.SANS'. The 'Merge' tab is selected, showing options for merging data. The 'Merge by Re-Binning [project]' button is highlighted. Below it, the 'Merge by Re-Binning [ascii]' button is also visible, along with a checkbox for 'Merge files within a row'. The 'binning of the Q-range' section has two options: 'Full Q-range [from datasets]' and 'Manual Q-Range'. The 'Manual Q-Range' option is selected, with 'Qmin: 0.0010' and 'Qmax: 0.3000' set. The 'skip points out of selected statistical-error range' section has a range from '0.00 %' to '100.00 %'. The 'after merging' section has 'remove first: 0 points' and 'remove last: 0 points'. The 'statistical equations behind...' section shows formulas for Q , dQ , I , dI , and Ω .

DAN.SANS

KWS1-2020

Options Rawdata Tools Mask Sensitivity Data Processing Merge

Merge

Merge by Re-Binning

... merging buttons: save as tables or ascii files

Merge by Re-Binning [project]

Merge by Re-Binning [ascii] ☐ Merge files within a row

... binning of the Q-range ...

☐ Full Q-range [from datasets] # Points: 300 ☒ Log.Step

☒ Manual Q-Range: Qmin: 0.0010 Qmax: 0.3000

... skip points out of selected statistical-error range ...

0.00 % ≤ Error ≤ 100.00 %

... after merging:

remove first: 0 points remove last: 0 points

... statistical equations behind...

$q, i, di, dq, \sigma \gg Q, I, dI, dQ, \Omega$

$Q = \Sigma q / N$ $dQ = \sqrt{(\Sigma dq^2) / N}$

$I = \Sigma i / N$ $dI = \sqrt{(\Sigma di^2) / N}$

$\Omega = (q_{max} - q_{min}) / 2 + \sqrt{(\Sigma \sigma^2) / N}$

DAN.SANS