

A Unified User-Friendly Instrument Control and Data

Acquisition System for the ORNL SANS Instrument Suite

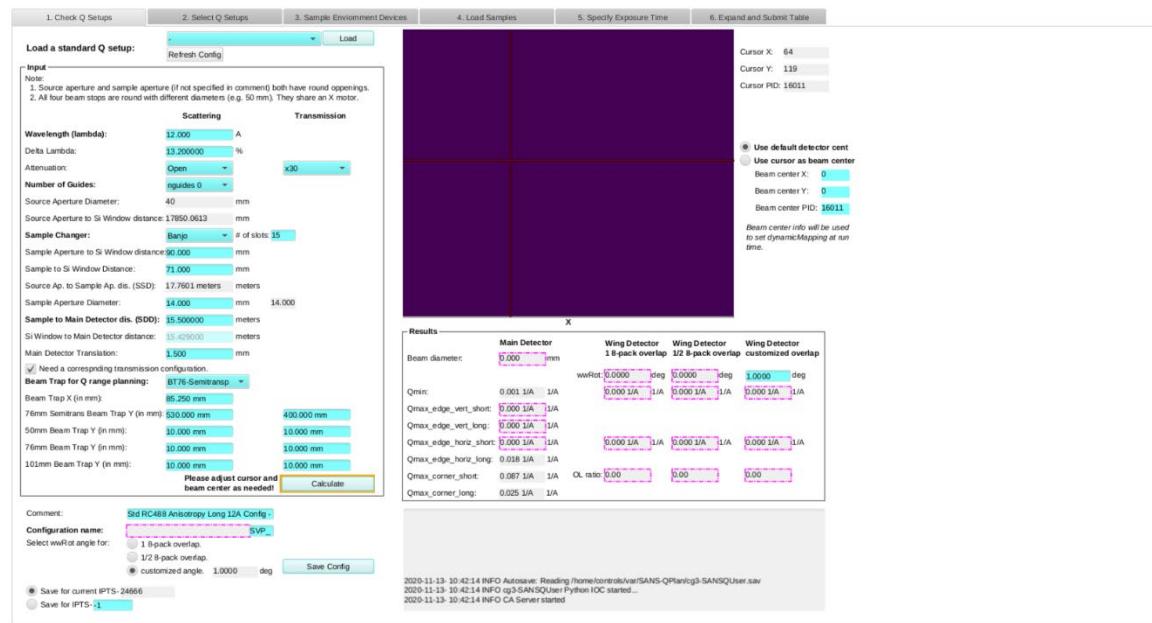
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This supplemental information presents screenshots for various tabs in the new system.

SANS Panel Scans



Load a standard Q setup: Refresh Config

Input

1. Source aperture and sample aperture (if not specified in comment) both have round openings.
2. All four beam stops are round with different diameters (e.g. 50 mm). They share an X motor.

Scattering Transmission

Wavelength (lambda): 12.0000 A

Delta Lambda: 13.200000 %

Attenuation: Open x30

Number of Guides: includes 0

Source Aperture Diameter: 40 mm

Source Aperture to Si Window distance: 1.7850.0633 mm

Sample Changer: Banjo a of slots: 15

Sample Aperture to Si Window distance: 90.000 mm

Sample to Si Window Distance: 71.000 mm

Source Ap to Sample Ap. dis. (SSD): 17.7601 meters meters

Sample Aperture Diameter: 14.000 mm 14.000 mm

Sample to Main Detector dis. (DD): 15.000000 meters

Si Window to Main Detector distance: 10.49000 meters

Main Detector Transition: 1.500 mm

Need a corresponding transmission configuration.

Beam Trap for Q range planning: BT7.5-Semitransp

Beam Trap X (in mm): 85.250 mm

76mm Semitrans Beam Trap Y (in mm): 30.000 mm 400.000 mm

50mm Beam Trap Y (in mm): 10.000 mm 10.000 mm

76mm Beam Trap Y (in mm): 10.000 mm 10.000 mm

101mm Beam Trap Y (in mm): 10.000 mm 10.000 mm

Please adjust cursor and beam center as needed!

Comment: SkRCA488 Antimony Long 12A Config

Configuration name: SVP

Select wvRot angle for: 1/8 pack overlap 1/2 8-pack overlap customized angle: 1.0000 deg

Save for current IPTS-24666 Save for IPTS-31

Results

Main Detector	Wing Detector	Wing Detector	Wing Detector	Wing Detector
Beam diameter:	0.000 mm	wvRot: 0.0000 deg	0.0000 deg	1.0000 deg
Qmin:	0.001 1/A	1/A	0.000 1/A	1/A
Qmax_edge_vert_short:	0.000 1/A	1/A	0.000 1/A	1/A
Qmax_edge_vert_long:	0.000 1/A	1/A	0.000 1/A	1/A
Qmax_edge_horiz_short:	0.000 1/A	1/A	0.000 1/A	1/A
Qmax_edge_horiz_long:	0.018 1/A	1/A	0.000 1/A	1/A
Qmax_corner_short:	0.087 1/A	1/A	0.000	0.00
Qmax_corner_long:	0.025 1/A	1/A	0.000	0.00

2020-11-13 10:42:14 INFO AutoSave: Reading /home/controls/avar/SANS-QPlaneg3-SANSQUser.sav
2020-11-13 10:42:14 INFO q3-SANSQUser: Python IOC started ...
2020-11-13 10:42:14 INFO CA Server started

Fig. S1 Check Q Setups tab in the Panel Scans interface. The yellow outline highlights buttons that are required to be clicked to ensure the output parameters to be calculated.

SANS Panel Scans

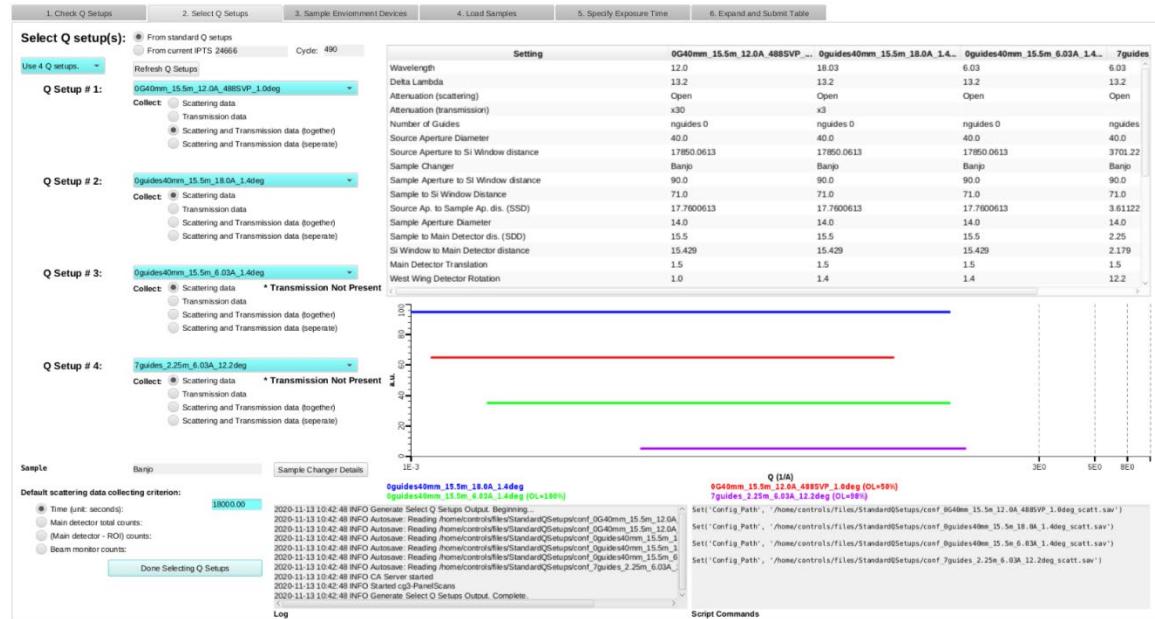


Fig. S2 Select Q Setups tab in the Panel Scans interface

SANS Panel Scans

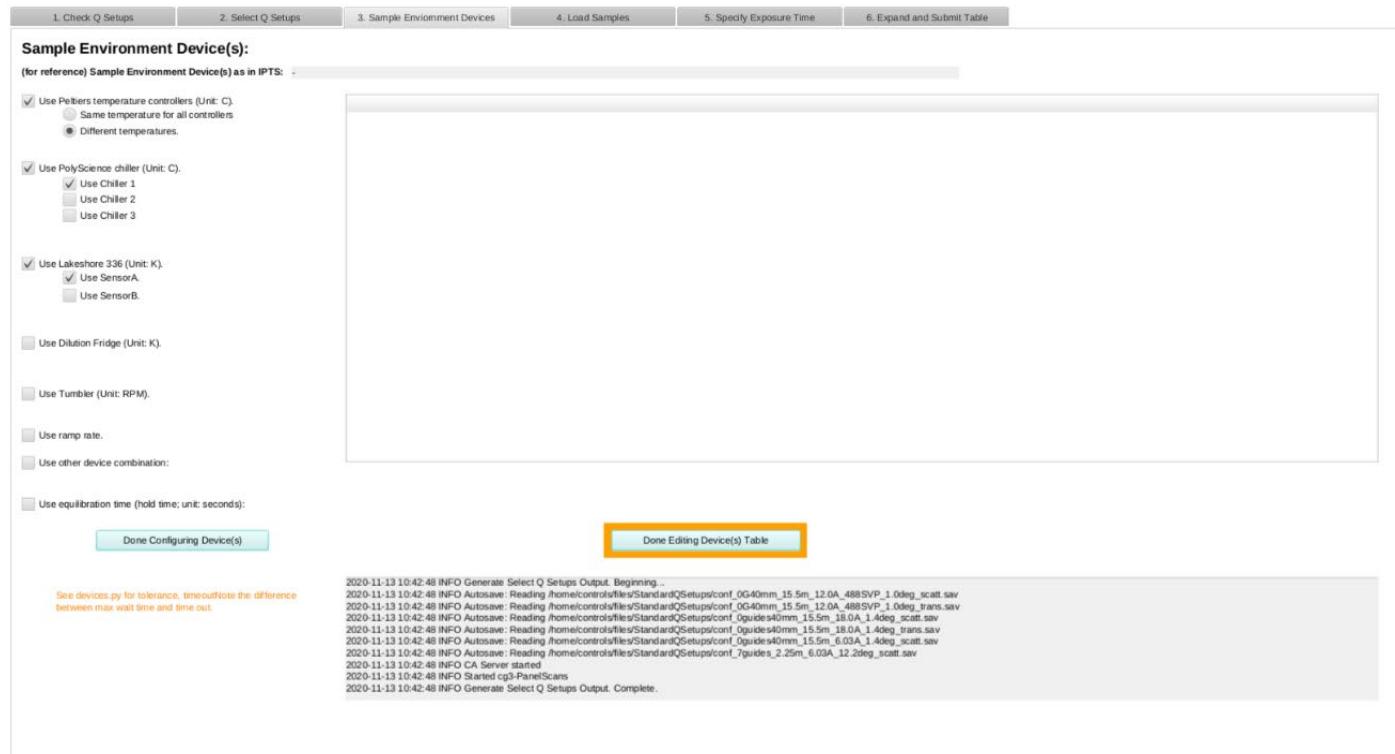


Fig. S3 Sample Environment Devices tab in the Panel Scans interface, for selecting specific sample environment for the current experiment. “Use other device combination:” will reveal the text input box to type a comma separated parameter names or aliases

SANS Panel Scans

1. Check Q Setups 2. Select Q Setups 3. Sample Environment Devices 4. Load Samples 5. Specify Exposure Time 6. Expand and Submit Table

Load Samples:

(for reference) Sample ID: 1 Sample Name: No sample

Sample Changer Default Positions to Use: 3-15 Edit Positions to Use: 1,5,7,9,13

Sample_Pos	Sample_Title	Sample_Thickness_mm	Composition	Composition_concentration	Solvent
Pos 1	s1				
Pos 5	s2				
Pos 7	s3				
Pos 9	s4				
Pos 13	s5				

Click to add row

Title

Background (e.g. "title within an experiment, run 1, run 2")

Sample thickness

Composition: protein (or polymer)

Default Composition: insp15

Composition concentration

Solvent

Default Solvent: 99mTc HEP

Solvent ratio

Salt

Salt concentration

Sample type (Sample/Background/Empty Cell/Open Beam)

Comment

[Done Configuring Sample Related Columns](#)

[Done Loading Sample Details](#)

```
2020-11-13 10:42:48 INFO Generate: Select Q Setups Output. Beginning.
2020-11-13 10:42:48 INFO Autowave: Reading /home/controls/files/Standard/QSetups/conf_0G40mm_15.5m_12.0A_488SVP_1.0deg_scatt.sav
2020-11-13 10:42:48 INFO Autowave: Reading /home/controls/files/Standard/QSetups/conf_0G40mm_15.5m_12.0A_488SVP_1.0deg_trans.sav
2020-11-13 10:42:48 INFO Autowave: Reading /home/controls/files/Standard/QSetups/conf_0guides40mm_15.5m_18.0A_1.4deg_trans.sav
2020-11-13 10:42:48 INFO Autowave: Reading /home/controls/files/Standard/QSetups/conf_0guides40mm_15.5m_18.0A_1.4deg_scatt.sav
2020-11-13 10:42:48 INFO Autowave: Reading /home/controls/files/Standard/QSetups/conf_0guides40mm_15.5m_6.03A_1.4deg_scatt.sav
2020-11-13 10:42:48 INFO Autowave: Reading /home/controls/files/Standard/QSetups/conf_7guides_2.25m_6.03A_12.2deg_scatt.sav
2020-11-13 10:42:48 INFO Autowave: Reading /home/controls/files/Standard/QSetups/conf_7guides_2.25m_6.03A_12.2deg_trans.sav
2020-11-13 10:42:48 INFO Started csgPanelScans
2020-11-13 10:42:48 INFO Generate: Select Q Setups Output. Complete.
```

Fig. S4 Load Samples tab in the Panel Scans interface, for more specific sample information

SANS Panel Scans

1. Check Q Setups 2. Select Q Setups 3. Sample Environment Devices 4. Load Samples 5. Specify Exposure Time 6. Expand and Submit Table

Specify Exposure Time:

Use max wait time (unit: seconds): 600.00

[Done Configuring - Generate Table](#)

Sample_Pos	Sample_Title	Config_Path	Wait For	Value	Or Time
Pos 1	s1	/home/controls/files/Standard/QSetups/conf_0G40mm_15.5m_12.0A_488SVP_1.0deg_scatt.sav	seconds	1800.0	600.0
Pos 1	s1	/home/controls/files/Standard/QSetups/conf_0guides40mm_15.5m_18.0A_1.4deg_scatt.sav	seconds	1800.0	600.0
Pos 1	s1	/home/controls/files/Standard/QSetups/conf_0guides40mm_15.5m_6.03A_1.4deg_scatt.sav	seconds	1800.0	600.0
Pos 1	s1	/home/controls/files/Standard/QSetups/conf_7guides_2.25m_6.03A_12.2deg_scatt.sav	seconds	1800.0	600.0
Pos 5	s2	/home/controls/files/Standard/QSetups/conf_0G40mm_15.5m_12.0A_488SVP_1.0deg_scatt.sav	seconds	1800.0	600.0
Pos 5	s2	/home/controls/files/Standard/QSetups/conf_0guides40mm_15.5m_18.0A_1.4deg_scatt.sav	seconds	1800.0	600.0
Pos 5	s2	/home/controls/files/Standard/QSetups/conf_0guides40mm_15.5m_6.03A_1.4deg_scatt.sav	seconds	1800.0	600.0
Pos 5	s2	/home/controls/files/Standard/QSetups/conf_7guides_2.25m_6.03A_12.2deg_scatt.sav	seconds	1800.0	600.0
Pos 7	s3	/home/controls/files/Standard/QSetups/conf_0G40mm_15.5m_12.0A_488SVP_1.0deg_scatt.sav	seconds	1800.0	600.0
Pos 7	s3	/home/controls/files/Standard/QSetups/conf_0guides40mm_15.5m_18.0A_1.4deg_scatt.sav	seconds	1800.0	600.0
Pos 7	s3	/home/controls/files/Standard/QSetups/conf_0guides40mm_15.5m_6.03A_1.4deg_scatt.sav	seconds	1800.0	600.0
Pos 7	s3	/home/controls/files/Standard/QSetups/conf_7guides_2.25m_6.03A_12.2deg_scatt.sav	seconds	1800.0	600.0
Pos 9	s4	/home/controls/files/Standard/QSetups/conf_0G40mm_15.5m_12.0A_488SVP_1.0deg_scatt.sav	seconds	1800.0	600.0
Pos 9	s4	/home/controls/files/Standard/QSetups/conf_0guides40mm_15.5m_18.0A_1.4deg_scatt.sav	seconds	1800.0	600.0
Pos 9	s4	/home/controls/files/Standard/QSetups/conf_0guides40mm_15.5m_6.03A_1.4deg_scatt.sav	seconds	1800.0	600.0
Pos 9	s4	/home/controls/files/Standard/QSetups/conf_7guides_2.25m_6.03A_12.2deg_scatt.sav	seconds	1800.0	600.0
Pos 13	s5	/home/controls/files/Standard/QSetups/conf_0guides40mm_15.5m_18.0A_1.4deg_scatt.sav	seconds	1800.0	600.0
Pos 13	s5	/home/controls/files/Standard/QSetups/conf_0guides40mm_15.5m_6.03A_1.4deg_scatt.sav	seconds	1800.0	600.0
Pos 13	s5	/home/controls/files/Standard/QSetups/conf_7guides_2.25m_6.03A_12.2deg_scatt.sav	seconds	1800.0	600.0

Click to add ...

```
2020-11-13 10:42:48 INFO Generate: Select Q Setups Output. Beginning.
2020-11-13 10:42:48 INFO Autowave: Reading /home/controls/files/Standard/QSetups/conf_0G40mm_15.5m_12.0A_488SVP_1.0deg_scatt.sav
2020-11-13 10:42:48 INFO Autowave: Reading /home/controls/files/Standard/QSetups/conf_0guides40mm_15.5m_18.0A_1.4deg_scatt.sav
2020-11-13 10:42:48 INFO Autowave: Reading /home/controls/files/Standard/QSetups/conf_0guides40mm_15.5m_6.03A_1.4deg_scatt.sav
2020-11-13 10:42:48 INFO Autowave: Reading /home/controls/files/Standard/QSetups/conf_7guides_2.25m_6.03A_12.2deg_scatt.sav
2020-11-13 10:42:48 INFO Autowave: Reading /home/controls/files/Standard/QSetups/conf_7guides_2.25m_6.03A_12.2deg_trans.sav
2020-11-13 10:42:48 INFO CA Server started
2020-11-13 10:42:48 INFO Started csgPanelScans
2020-11-13 10:42:48 INFO Generate: Select Q Setups Output. Complete.
```

[Done Editing Exposure Time Table](#)

Fig. S5 Specify Exposure Time tab in the Panel Scans interface to setup measurement time or detector count at different configurations and samples

SANS Panel Scans

1. Check Q Setups 2. Select Q Setups 3. Sample Environment Devices 4. Load Samples 5. Specify Exposure Time 6. Expand and Submit Table

Expand Order:

- Sample env settings, Q setups (scattering first), sample positions
- Sample env settings, Q setups (transmission first), sample positions
- Q setups (scattering first), sample env settings, sample positions.
- Q setups (transmission first), sample env settings, sample positions.
- Sample positions, Q setups (scattering first), sample env settings.
- Sample env settings, sample positions, Q setups (scattering first).

Panel Scan Protocols:

Title	Config_Path	Measure_Type	Sample_Pos	Sample_Title	Sample_Thickness_mm	Composition	Composition_concentration
Panel Scan 1 of 20, smpl: s1	home/controls/files/Standar dQSetup/Conf_0G40mm_15.5m_12.0A_488SVP_1.0deg_scatt.sav	Both	Pos 1	s1	nsp15	50 mM HEPES, 1	
Panel Scan 2 of 20, smpl: s2	home/controls/files/Standar dQSetup/Conf_0G40mm_15.5m_12.0A_488SVP_1.0deg_scatt.sav	Both	Pos 5	s1	nsp15	50 mM HEPES, 1	
Panel Scan 3 of 20, smpl: s3	home/controls/files/Standar dQSetup/Conf_0G40mm_15.5m_12.0A_488SVP_1.0deg_scatt.sav	Both	Pos 7	s3	nsp15	50 mM HEPES, 1	
Panel Scan 4 of 20, smpl: s4	home/controls/files/Standar dQSetup/Conf_0G40mm_15.5m_12.0A_488SVP_1.0deg_scatt.sav	Both	Pos 9	s4	nsp15	50 mM HEPES, 1	
Panel Scan 5 of 20, smpl: s5	home/controls/files/Standar dQSetup/Conf_0G40mm_15.5m_12.0A_488SVP_1.0deg_scatt.sav	Both	Pos 13	s5	nsp15	50 mM HEPES, 1	
Panel Scan 6 of 20, smpl: s1	home/controls/files/Standar dQSetup/Conf_0Quide40mm_15.5m_18.0A_1.4deg_scatt.sav	Scattering	Pos 1	s1	nsp15	50 mM HEPES, 1	
Panel Scan 7 of 20, smpl: s2	home/controls/files/Standar dQSetup/Conf_0Quide40mm_15.5m_18.0A_1.4deg_scatt.sav	Scattering	Pos 5	s2	nsp15	50 mM HEPES, 1	
Panel Scan 8 of 20, smpl: s3	home/controls/files/Standar dQSetup/Conf_0Quide40mm_15.5m_18.0A_1.4deg_scatt.sav	Scattering	Pos 7	s3	nsp15	50 mM HEPES, 1	
Panel Scan 9 of 20, smpl: s4	home/controls/files/Standar dQSetup/Conf_0Quide40mm_15.5m_18.0A_1.4deg_scatt.sav	Scattering	Pos 9	s4	nsp15	50 mM HEPES, 1	
Panel Scan 10 of 20, smpl: s5	home/controls/files/Standar dQSetup/Conf_0Quide40mm_15.5m_18.0A_1.4deg_scatt.sav	Scattering	Pos 13	s5	nsp15	50 mM HEPES, 1	
Panel Scan 11 of 20, smpl: s1	home/controls/files/Standar dQSetup/Conf_0Quide40mm_15.5m_6.0A_1.4deg_scatt.sav	Scattering	Pos 1	s1	nsp15	50 mM HEPES, 1	
Panel Scan 12 of 20, smpl: s2	home/controls/files/Standar dQSetup/Conf_0Quide40mm_15.5m_6.0A_1.4deg_scatt.sav	Scattering	Pos 5	s2	nsp15	50 mM HEPES, 1	
Panel Scan 13 of 20, smpl: s3	home/controls/files/Standar dQSetup/Conf_0Quide40mm_15.5m_6.0A_1.4deg_scatt.sav	Scattering	Pos 7	s3	nsp15	50 mM HEPES, 1	
Panel Scan 14 of 20, smpl: s4	home/controls/files/Standar dQSetup/Conf_0Quide40mm_15.5m_6.0A_1.4deg_scatt.sav	Scattering	Pos 9	s4	nsp15	50 mM HEPES, 1	
Panel Scan 15 of 20, smpl: s5	home/controls/files/Standar dQSetup/Conf_0Quide40mm_15.5m_6.0A_1.4deg_scatt.sav	Scattering	Pos 13	s5	nsp15	50 mM HEPES, 1	
Panel Scan 16 of 20, smpl: s1	home/controls/files/Standar dQSetup/Conf_7guides_2.25m_6.03A_12.2deg_scatt.sav	Scattering	Pos 1	s1	nsp15	50 mM HEPES, 1	
Panel Scan 17 of 20, smpl: s2	home/controls/files/Standar dQSetup/Conf_7guides_2.25m_6.03A_12.2deg_scatt.sav	Scattering	Pos 5	s2	nsp15	50 mM HEPES, 1	
Panel Scan 18 of 20, smpl: s3	home/controls/files/Standar dQSetup/Conf_7guides_2.25m_6.03A_12.2deg_scatt.sav	Scattering	Pos 7	s3	nsp15	50 mM HEPES, 1	
Panel Scan 19 of 20, smpl: s4	home/controls/files/Standar dQSetup/Conf_7guides_2.25m_6.03A_12.2deg_scatt.sav	Scattering	Pos 9	s4	nsp15	50 mM HEPES, 1	
Panel Scan 20 of 20, smpl: s5	home/controls/files/Standar dQSetup/Conf_7guides_2.25m_6.03A_12.2deg_scatt.sav	Scattering	Pos 13	s5	nsp15	50 mM HEPES, 1	
Unset			Undefined	Out	Undefined	Undefined	Undefined

Click to add row

2020-11-13 10:42:48 INFO Generic: Select Q Setups Output. Beginning.
2020-11-13 10:42:48 INFO Autosave: Reading /home/controls/files/Standar dQSetup/Conf_0G40mm_15.5m_12.0A_488SVP_1.0deg_scatt.sav
2020-11-13 10:42:48 INFO Autosave: Reading /home/controls/files/Standar dQSetup/Conf_0G40mm_15.5m_12.0A_488SVP_1.0deg_trans.sav
2020-11-13 10:42:48 INFO Autosave: Reading /home/controls/files/Standar dQSetup/Conf_0Quide40mm_15.5m_18.0A_1.4deg_scatt.sav
2020-11-13 10:42:48 INFO Autosave: Reading /home/controls/files/Standar dQSetup/Conf_0Quide40mm_15.5m_6.0A_1.4deg_scatt.sav
2020-11-13 10:42:48 INFO Autosave: Reading /home/controls/files/Standar dQSetup/Conf_7guides_2.25m_6.03A_12.2deg_scatt.sav
2020-11-13 10:42:48 INFO Autosave: Reading /home/controls/files/Standar dQSetup/Conf_7guides_2.25m_6.03A_12.2deg_trans.sav
2020-11-13 10:42:48 INFO Started cgs-PanelScans
2020-11-13 10:42:48 INFO Generic Select Q Setups Output. Complete.

Total Rows: 22 Submit Separate Scan Jobs Simulate
Delay Sum: 0.00 Submit One Scan Job Save Table File
Value Sum: 360000.00
Table file name: /home/controls/var/tmp/ScanMotor_UsingAlignScan_Th

Fig. S6 Expand and Submit tab in the Panel Scans interface. It expands the scans in different ways with all conditions from previous setups (such as samples, sample environment, configurations, measurement type (transmission, scattering or both)), only part of the columns are shown in the screenshot

SANS Q Planner

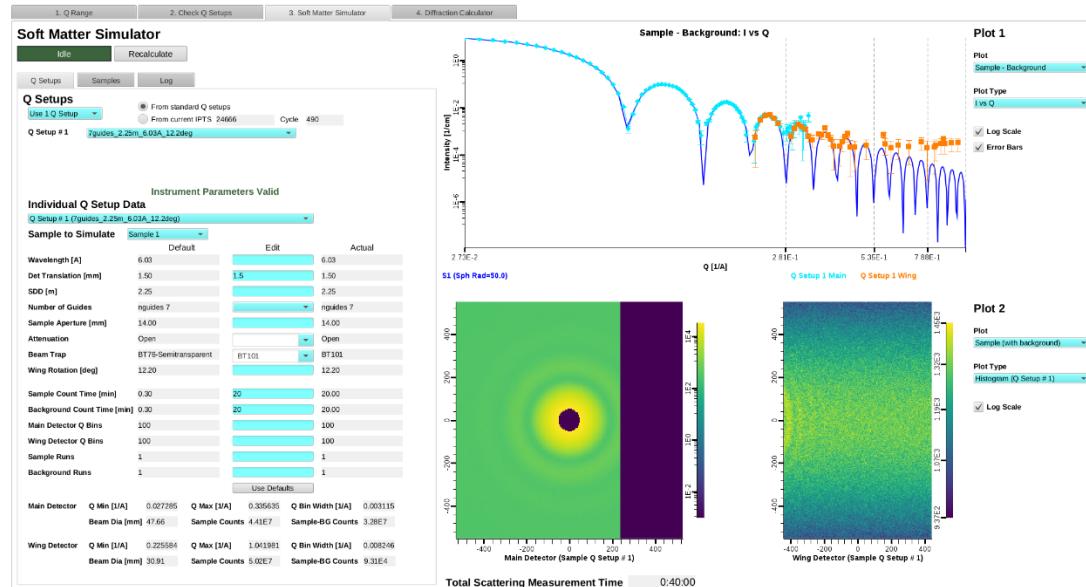


Fig. S7 The soft matter simulator with instrument specific parameters