

# 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

The screenshot displays the 'SANS Panel Scans' interface, specifically the 'Check Q Setups' tab. The interface is organized into several sections:

- Top Navigation:** A series of tabs labeled 1. Check Q Setups, 2. Select Q Setups, 3. Sample Environment Devices, 4. Load Samples, 5. Specify Exposure Time, and 6. Expand and Submit Table.
- Input Section:** Contains fields for 'Load a standard Q setup:' (with a 'Refresh Config' button), 'Input' (with a 'Load' button), and various parameters for scattering and transmission. Parameters include Wavelength (lambda), Delta Lambda, Attenuation, Number of Guides, Source Aperture Diameter, Source Aperture to Si Window distance, Sample Changer, Sample Aperture to Si Window distance, Sample to Si Window Distance, Source Ap. to Sample Ap. dis. (SSD), Sample Aperture Diameter, Sample to Main Detector dis. (SDD), Si Window to Main Detector distance, Main Detector Translation, and a checkbox for 'Need a corresponding transmission configuration'.
- Beam Trap for Q range planning:** A section with a dropdown menu and input fields for beam trap dimensions (X, Y, Z) for different beam sizes (76mm, 50mm, 10mm, 100mm).
- Comment and Configuration:** A text area for comments, a 'Configuration name' field, and radio buttons for '1/2 8-pack overlap', '1/2 8-pack overlap', and 'customized angle'.
- Results Section:** A table showing parameters for the Main Detector and three Wing Detectors. Parameters include Beam diameter, Wavelength, Qmin, Qmax (edge, corner, short, long), and OL ratio.
- Buttons:** A yellow outline highlights the 'Calculate' button and the 'Save Config' button.

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

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

**Select Q setup(s):** ☒ From standard Q setups ☐ From current IPTS 24666 Cycle: 490

Use 4 Q setups Refresh Q Setups

**Q Setup # 1:** **OG40mm\_15.5m\_12.0A\_488SVP\_1.0deg**

Collect: ☒ Scattering data ☐ Transmission data ☐ Scattering and Transmission data (together) ☐ Scattering and Transmission data (separate)

**Q Setup # 2:** **OG40mm\_15.5m\_18.0A\_1.4deg**

Collect: ☒ Scattering data ☐ Transmission data ☐ Scattering and Transmission data (together) ☐ Scattering and Transmission data (separate)

**Q Setup # 3:** **OG40mm\_15.5m\_6.03A\_1.4deg**

Collect: ☒ Scattering data ☐ Transmission data ☐ Scattering and Transmission data (together) ☐ Scattering and Transmission data (separate)

**Q Setup # 4:** **7guides\_2.25m\_6.03A\_12.2deg**

Collect: ☒ Scattering data ☐ Transmission data ☐ Scattering and Transmission data (together) ☐ Scattering and Transmission data (separate)

**Sample** Bangs Sample Changer Details

Default scattering data collecting criterion: 18000.00

☒ Time (unit: seconds) ☐ Main detector total counts ☐ Main detector - HDI counts ☐ Beam monitor counts

Done Selecting Q Setups

2020-11-13 10:42:48 INFO Generate Select Q Setups Output. Beginning...

2020-11-13 10:42:48 INFO Autosave: Reading /home/control/files/StandardQSetups/conf\_OG40mm\_15.5m\_12.0A\_488SVP\_1.0deg\_scatt.sav

2020-11-13 10:42:48 INFO Autosave: Reading /home/control/files/StandardQSetups/conf\_OG40mm\_15.5m\_18.0A\_1.4deg\_scatt.sav

2020-11-13 10:42:48 INFO Autosave: Reading /home/control/files/StandardQSetups/conf\_OG40mm\_15.5m\_6.03A\_1.4deg\_scatt.sav

2020-11-13 10:42:48 INFO Autosave: Reading /home/control/files/StandardQSetups/conf\_7guides\_2.25m\_6.03A\_12.2deg\_scatt.sav

2020-11-13 10:42:48 INFO CA Server started

2020-11-13 10:42:48 INFO Started csg-PanelScans

2020-11-13 10:42:48 INFO Generate Select Q Setups Output. Complete.

Log

Script Commands

Set! 'Config.Path' - '/home/control/files/StandardQSetups/conf\_OG40mm\_15.5m\_12.0A\_488SVP\_1.0deg\_scatt.sav'

Set! 'Config.Path' - '/home/control/files/StandardQSetups/conf\_OG40mm\_15.5m\_18.0A\_1.4deg\_scatt.sav'

Set! 'Config.Path' - '/home/control/files/StandardQSetups/conf\_OG40mm\_15.5m\_6.03A\_1.4deg\_scatt.sav'

Set! 'Config.Path' - '/home/control/files/StandardQSetups/conf\_7guides\_2.25m\_6.03A\_12.2deg\_scatt.sav'

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

## 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

**Sample Environment Device(s):**

(for reference) Sample Environment Device(s) as in IPTS: -

☒ Use Peltiers temperature controllers (Unit: C): ☐ Same temperature for all controllers ☒ Different temperatures.

☒ Use PolyScience chiller (Unit: C): ☒ Use Chiller 1 ☐ Use Chiller 2 ☐ Use Chiller 3

☒ Use Lakeshore 336 (Unit: K): ☒ Use SensorA ☐ Use SensorB.

☐ Use Dilution Fridge (Unit: K).

☐ Use Tumbler (Unit: RPM).

☐ Use ramp rate.

☐ Use other device combination:

☐ Use equilibration time (hold time; unit: seconds):

Done Configuring Device(s)

Done Editing Device(s) Table

See devices.py for tolerance, timeout into the difference between max wait time and time out.

2020-11-13 10:42:48 INFO Generate Select Q Setups Output. Beginning...

2020-11-13 10:42:48 INFO Autosave: Reading /home/control/files/StandardQSetups/conf\_OG40mm\_15.5m\_12.0A\_488SVP\_1.0deg\_scatt.sav

2020-11-13 10:42:48 INFO Autosave: Reading /home/control/files/StandardQSetups/conf\_OG40mm\_15.5m\_12.0A\_488SVP\_1.0deg\_trans.sav

2020-11-13 10:42:48 INFO Autosave: Reading /home/control/files/StandardQSetups/conf\_OG40mm\_15.5m\_18.0A\_1.4deg\_scatt.sav

2020-11-13 10:42:48 INFO Autosave: Reading /home/control/files/StandardQSetups/conf\_OG40mm\_15.5m\_18.0A\_1.4deg\_trans.sav

2020-11-13 10:42:48 INFO Autosave: Reading /home/control/files/StandardQSetups/conf\_OG40mm\_15.5m\_6.03A\_1.4deg\_scatt.sav

2020-11-13 10:42:48 INFO Autosave: Reading /home/control/files/StandardQSetups/conf\_7guides\_2.25m\_6.03A\_12.2deg\_scatt.sav

2020-11-13 10:42:48 INFO CA Server started

2020-11-13 10:42:48 INFO Started csg-PanelScans

2020-11-13 10:42:48 INFO Generate Select Q Setups Output. Complete.

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

**Load Samples:**

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

☒ Sample Changer Default Positions to Use: 1-35 Edit Positions to Use:

☐ ITEMS IDs

☒ Title

☐ Background (If g. Title within an experiment, run1, run2)

☒ Sample thickness

☒ Composition: protein (or polymer) Default Composition:

☒ Composition concentration

☒ Solvent Default Solvent:

☐ 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 Setup Output. Beginning...

2020-11-13 10:42:48 INFO Autosave: Reading home/control/files/StandardQSetup/conf\_0G40mm\_15.5m\_12.0A\_488SVP\_1.0deg\_scatt.sav

2020-11-13 10:42:48 INFO Autosave: Reading home/control/files/StandardQSetup/conf\_0G40mm\_15.5m\_12.0A\_488SVP\_1.0deg\_trans.sav

2020-11-13 10:42:48 INFO Autosave: Reading home/control/files/StandardQSetup/conf\_0guides40mm\_15.5m\_18.0A\_1.4deg\_scatt.sav

2020-11-13 10:42:48 INFO Autosave: Reading home/control/files/StandardQSetup/conf\_0guides40mm\_15.5m\_18.0A\_1.4deg\_trans.sav

2020-11-13 10:42:48 INFO Autosave: Reading home/control/files/StandardQSetup/conf\_7guides\_2.25m\_6.03A\_12.2deg\_scatt.sav

2020-11-13 10:42:48 INFO Autosave: Reading home/control/files/StandardQSetup/conf\_7guides\_2.25m\_6.03A\_12.2deg\_scatt.sav

2020-11-13 10:42:48 INFO CA Server started

2020-11-13 10:42:48 INFO Started up3-PanelScans

2020-11-13 10:42:48 INFO Generate Select Q Setup Output. Complete.

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

## SANS Panel Scans

1. Check Q Setup
2. Select Q Setup
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):

Done Configuring - Generate Table

Sample_Pos	Sample_Title	Config_Path	Wait_For	Value	Or_Time
Pos 1	s1	home/control/files/StandardQSetup/conf_0G40mm_15.5m_12.0A_488SVP_1.0deg_scatt.sav	seconds	18000.0	600.0
Pos 1	s1	home/control/files/StandardQSetup/conf_0guides40mm_15.5m_18.0A_1.4deg_scatt.sav	seconds	18000.0	600.0
Pos 1	s1	home/control/files/StandardQSetup/conf_7guides_2.25m_6.03A_12.2deg_scatt.sav	seconds	18000.0	600.0
Pos 5	s2	home/control/files/StandardQSetup/conf_0G40mm_15.5m_12.0A_488SVP_1.0deg_scatt.sav	seconds	18000.0	600.0
Pos 5	s2	home/control/files/StandardQSetup/conf_0guides40mm_15.5m_18.0A_1.4deg_scatt.sav	seconds	18000.0	600.0
Pos 5	s2	home/control/files/StandardQSetup/conf_0guides40mm_15.5m_6.03A_1.4deg_scatt.sav	seconds	18000.0	600.0
Pos 5	s2	home/control/files/StandardQSetup/conf_7guides_2.25m_6.03A_12.2deg_scatt.sav	seconds	18000.0	600.0
Pos 7	s3	home/control/files/StandardQSetup/conf_0G40mm_15.5m_12.0A_488SVP_1.0deg_scatt.sav	seconds	18000.0	600.0
Pos 7	s3	home/control/files/StandardQSetup/conf_0guides40mm_15.5m_18.0A_1.4deg_scatt.sav	seconds	18000.0	600.0
Pos 7	s3	home/control/files/StandardQSetup/conf_7guides_2.25m_6.03A_12.2deg_scatt.sav	seconds	18000.0	600.0
Pos 9	s4	home/control/files/StandardQSetup/conf_0G40mm_15.5m_12.0A_488SVP_1.0deg_scatt.sav	seconds	18000.0	600.0
Pos 9	s4	home/control/files/StandardQSetup/conf_0guides40mm_15.5m_18.0A_1.4deg_scatt.sav	seconds	18000.0	600.0
Pos 9	s4	home/control/files/StandardQSetup/conf_0guides40mm_15.5m_6.03A_1.4deg_scatt.sav	seconds	18000.0	600.0
Pos 9	s4	home/control/files/StandardQSetup/conf_7guides_2.25m_6.03A_12.2deg_scatt.sav	seconds	18000.0	600.0
Pos 13	s5	home/control/files/StandardQSetup/conf_0G40mm_15.5m_12.0A_488SVP_1.0deg_scatt.sav	seconds	18000.0	600.0
Pos 13	s5	home/control/files/StandardQSetup/conf_0guides40mm_15.5m_18.0A_1.4deg_scatt.sav	seconds	18000.0	600.0
Pos 13	s5	home/control/files/StandardQSetup/conf_0guides40mm_15.5m_6.03A_1.4deg_scatt.sav	seconds	18000.0	600.0
Pos 13	s5	home/control/files/StandardQSetup/conf_7guides_2.25m_6.03A_12.2deg_scatt.sav	seconds	18000.0	600.0

Click to add ...

2020-11-13 10:42:48 INFO Generate Select Q Setup Output. Beginning...

2020-11-13 10:42:48 INFO Autosave: Reading home/control/files/StandardQSetup/conf\_0G40mm\_15.5m\_12.0A\_488SVP\_1.0deg\_scatt.sav

2020-11-13 10:42:48 INFO Autosave: Reading home/control/files/StandardQSetup/conf\_0G40mm\_15.5m\_12.0A\_488SVP\_1.0deg\_trans.sav

2020-11-13 10:42:48 INFO Autosave: Reading home/control/files/StandardQSetup/conf\_0guides40mm\_15.5m\_18.0A\_1.4deg\_scatt.sav

2020-11-13 10:42:48 INFO Autosave: Reading home/control/files/StandardQSetup/conf\_0guides40mm\_15.5m\_18.0A\_1.4deg\_trans.sav

2020-11-13 10:42:48 INFO Autosave: Reading home/control/files/StandardQSetup/conf\_7guides\_2.25m\_6.03A\_12.2deg\_scatt.sav

2020-11-13 10:42:48 INFO Autosave: Reading home/control/files/StandardQSetup/conf\_7guides\_2.25m\_6.03A\_12.2deg\_scatt.sav

2020-11-13 10:42:48 INFO CA Server started

2020-11-13 10:42:48 INFO Started up3-PanelScans

2020-11-13 10:42:48 INFO Generate Select Q Setup 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

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).

Title	Config_Path	Measure_Type	Sample_Pos	Sample_Title	Sample_Thickness_nm	Composition	Composition_concentration
Panel Scan Protocol							
Panel Scan 1 of 20, smpl: s1	/home/controler/files/StandardQSetup/conf_QG40mm_15_5m_12.0A_48BSVP_1.0deg_scatt.sav	Both	Pos 1	s1		nps15	50 mM HEPES, 1
Panel Scan 2 of 20, smpl: s2	/home/controler/files/StandardQSetup/conf_QG40mm_15_5m_12.0A_48BSVP_1.0deg_scatt.sav	Both	Pos 5	s2		nps15	50 mM HEPES, 1
Panel Scan 3 of 20, smpl: s3	/home/controler/files/StandardQSetup/conf_QG40mm_15_5m_12.0A_48BSVP_1.0deg_scatt.sav	Both	Pos 7	s3		nps15	50 mM HEPES, 1
Panel Scan 4 of 20, smpl: s4	/home/controler/files/StandardQSetup/conf_QG40mm_15_5m_12.0A_48BSVP_1.0deg_scatt.sav	Both	Pos 9	s4		nps15	50 mM HEPES, 1
Panel Scan 5 of 20, smpl: s5	/home/controler/files/StandardQSetup/conf_QG40mm_15_5m_12.0A_48BSVP_1.0deg_scatt.sav	Both	Pos 13	s5		nps15	50 mM HEPES, 1
Panel Scan 6 of 20, smpl: s1	/home/controler/files/StandardQSetup/conf_QGides40mm_15_15m_18.0A_1.4deg_scatt.sav	Scattering	Pos 1	s1		nps15	50 mM HEPES, 1
Panel Scan 7 of 20, smpl: s2	/home/controler/files/StandardQSetup/conf_QGides40mm_15_15m_18.0A_1.4deg_scatt.sav	Scattering	Pos 5	s2		nps15	50 mM HEPES, 1
Panel Scan 8 of 20, smpl: s3	/home/controler/files/StandardQSetup/conf_QGides40mm_15_15m_18.0A_1.4deg_scatt.sav	Scattering	Pos 7	s3		nps15	50 mM HEPES, 1
Panel Scan 9 of 20, smpl: s4	/home/controler/files/StandardQSetup/conf_QGides40mm_15_15m_18.0A_1.4deg_scatt.sav	Scattering	Pos 9	s4		nps15	50 mM HEPES, 1
Panel Scan 10 of 20, smpl: s5	/home/controler/files/StandardQSetup/conf_QGides40mm_15_15m_18.0A_1.4deg_scatt.sav	Scattering	Pos 13	s5		nps15	50 mM HEPES, 1
Panel Scan 11 of 20, smpl: s1	/home/controler/files/StandardQSetup/conf_QGides40mm_15_5m_6.03A_1.4deg_scatt.sav	Scattering	Pos 1	s1		nps15	50 mM HEPES, 1
Panel Scan 12 of 20, smpl: s2	/home/controler/files/StandardQSetup/conf_QGides40mm_15_5m_6.03A_1.4deg_scatt.sav	Scattering	Pos 5	s2		nps15	50 mM HEPES, 1
Panel Scan 13 of 20, smpl: s3	/home/controler/files/StandardQSetup/conf_QGides40mm_15_5m_6.03A_1.4deg_scatt.sav	Scattering	Pos 7	s3		nps15	50 mM HEPES, 1
Panel Scan 14 of 20, smpl: s4	/home/controler/files/StandardQSetup/conf_QGides40mm_15_5m_6.03A_1.4deg_scatt.sav	Scattering	Pos 9	s4		nps15	50 mM HEPES, 1
Panel Scan 15 of 20, smpl: s5	/home/controler/files/StandardQSetup/conf_QGides40mm_15_5m_6.03A_1.4deg_scatt.sav	Scattering	Pos 13	s5		nps15	50 mM HEPES, 1
Panel Scan 16 of 20, smpl: s1	/home/controler/files/StandardQSetup/conf_Tguides_2.25m_6.03A_12.2deg_scatt.sav	Scattering	Pos 1	s1		nps15	50 mM HEPES, 1
Panel Scan 17 of 20, smpl: s2	/home/controler/files/StandardQSetup/conf_Tguides_2.25m_6.03A_12.2deg_scatt.sav	Scattering	Pos 5	s2		nps15	50 mM HEPES, 1
Panel Scan 18 of 20, smpl: s3	/home/controler/files/StandardQSetup/conf_Tguides_2.25m_6.03A_12.2deg_scatt.sav	Scattering	Pos 7	s3		nps15	50 mM HEPES, 1
Panel Scan 19 of 20, smpl: s4	/home/controler/files/StandardQSetup/conf_Tguides_2.25m_6.03A_12.2deg_scatt.sav	Scattering	Pos 9	s4		nps15	50 mM HEPES, 1
Panel Scan 20 of 20, smpl: s5	/home/controler/files/StandardQSetup/conf_Tguides_2.25m_6.03A_12.2deg_scatt.sav	Scattering	Pos 13	s5		nps15	50 mM HEPES, 1
Unset		Undefined	Out	Undefined		Undefined	Undefined

Click to add row

2020-11-13 10:42:48 INFO Generate: Select Q Setups Output, Beginning...

2020-11-13 10:42:48 INFO Autotune: Reading /home/controler/files/StandardQSetup/conf\_QG40mm\_15\_5m\_12.0A\_48BSVP\_1.0deg\_scatt.sav

2020-11-13 10:42:48 INFO Autotune: Reading /home/controler/files/StandardQSetup/conf\_QG40mm\_15\_5m\_12.0A\_48BSVP\_1.0deg\_trans.sav

2020-11-13 10:42:48 INFO Autotune: Reading /home/controler/files/StandardQSetup/conf\_QGides40mm\_15\_15m\_18.0A\_1.4deg\_scatt.sav

2020-11-13 10:42:48 INFO Autotune: Reading /home/controler/files/StandardQSetup/conf\_QGides40mm\_15\_15m\_18.0A\_1.4deg\_trans.sav

2020-11-13 10:42:48 INFO Autotune: Reading /home/controler/files/StandardQSetup/conf\_QGides40mm\_15\_5m\_6.03A\_1.4deg\_scatt.sav

2020-11-13 10:42:48 INFO Autotune: Reading /home/controler/files/StandardQSetup/conf\_Tguides\_2.25m\_6.03A\_12.2deg\_scatt.sav

2020-11-13 10:42:48 INFO CA Server started

2020-11-13 10:42:48 INFO Started up PanelScans

2020-11-13 10:42:48 INFO Generate Select Q Setups Output, Complete.

Total Rows: 22

Delay Sum: 0.00

Value Sum: 360000.00

Table file name: /home/controler/var/ScanMotor\_UshingArgonScan\_Th

## SANS O Planner

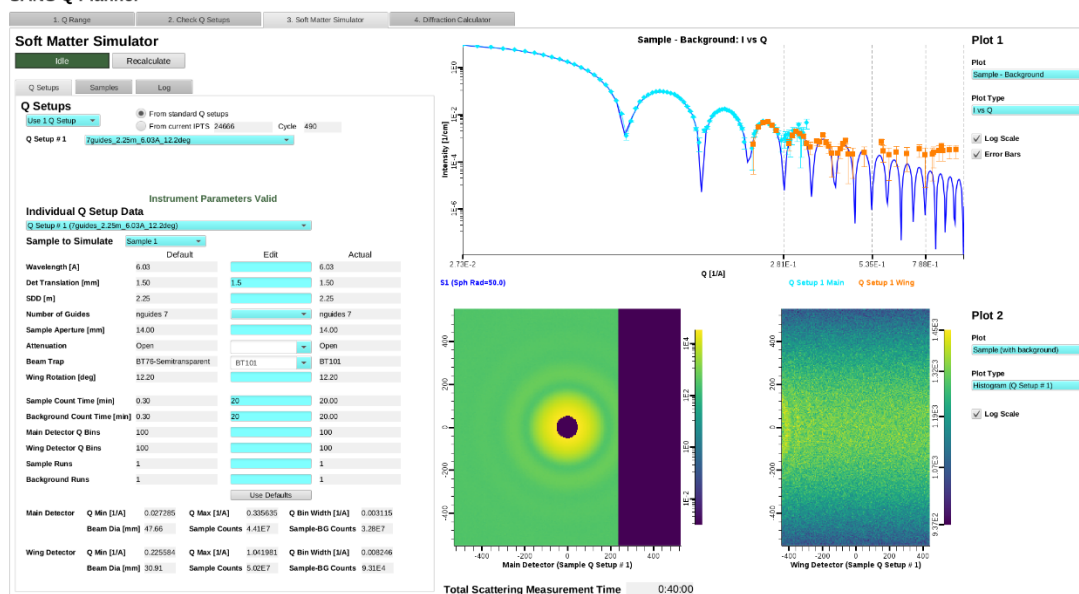


Fig. S7 The soft matter simulator with instrument specific parameters