

Automation at Upgraded SER-CAT

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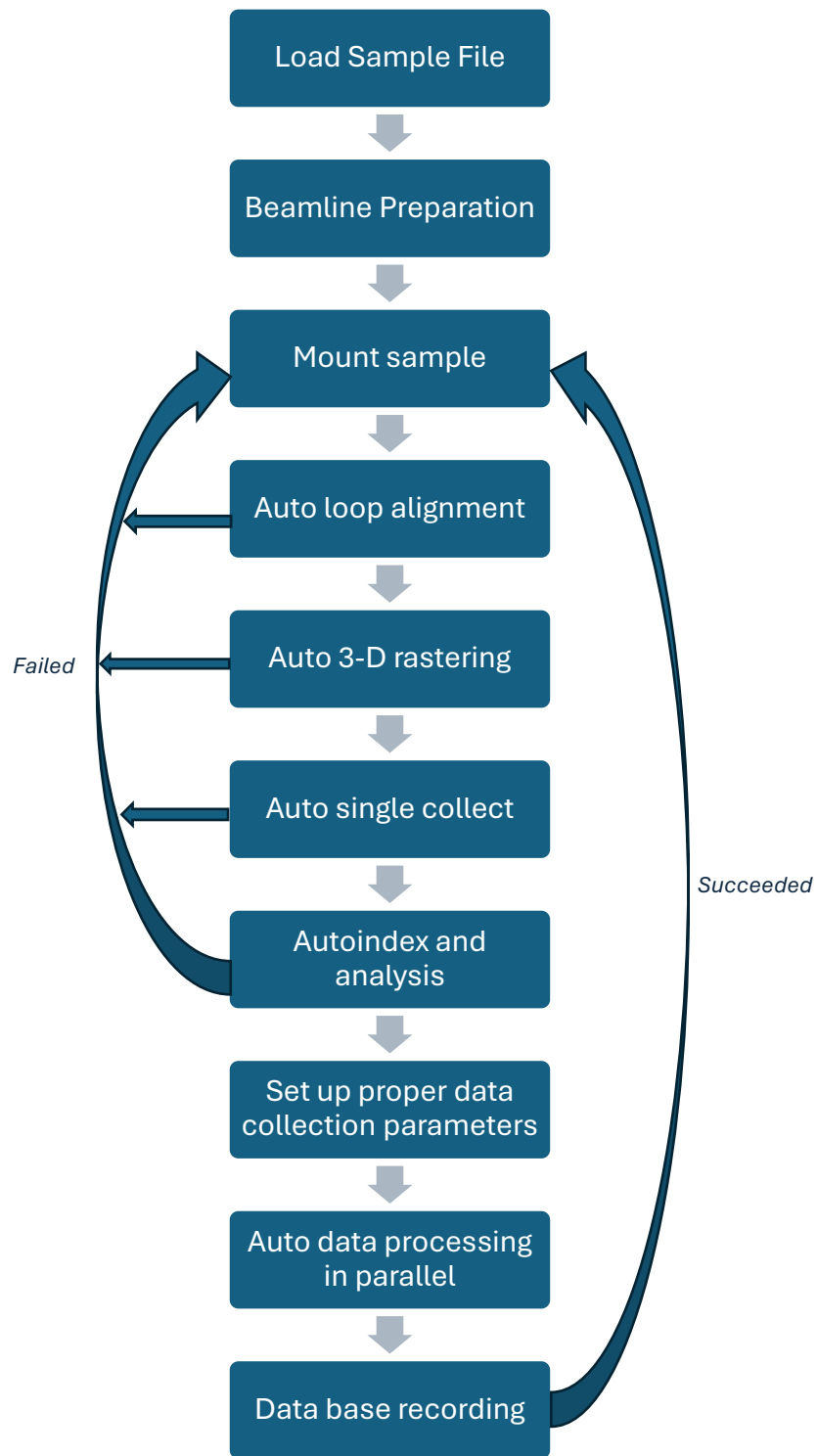
The upgraded SER-CAT 22ID-D beamline now delivers a stable, bright X-ray beam with a 30 μm x 30 μm spot size and a flux of 3×10^{13} photons/s at the sample position. The beamline provides monochromatic X-ray energies from 6–18 keV. A newly installed FMB double-crystal monochromator equipped with Si(111) and Si(220) crystal pairs enables users to optimize either flux or energy resolution to meet diverse experimental requirements. A new MD3 micro-diffractometer, upgraded sample-handling robot, and enhanced detector support provide fast, reliable, and flexible capabilities for macromolecular crystallography. The robotic system accommodates up to 30 UniPucks, with 20 full pucks available for simultaneous setup, enabling efficient support for multiple user groups.

The SER-CAT beamline control and data-collection interface, SERGUI2, has been redesigned to provide powerful tools for remote SAD, MAD, and other crystallographic experiments. A fully automated data-collection pipeline has been developed and extensively tested. Using user-supplied sample files, the automation system executes all marked samples through a sequence of operations including:

- sample mounting
- autoloop alignment
- 3-D rastering
- single-image screening
- auto-indexing and quality assessment
- automated transmission and exposure optimization
- automated data collection
- automated data processing
- database recording

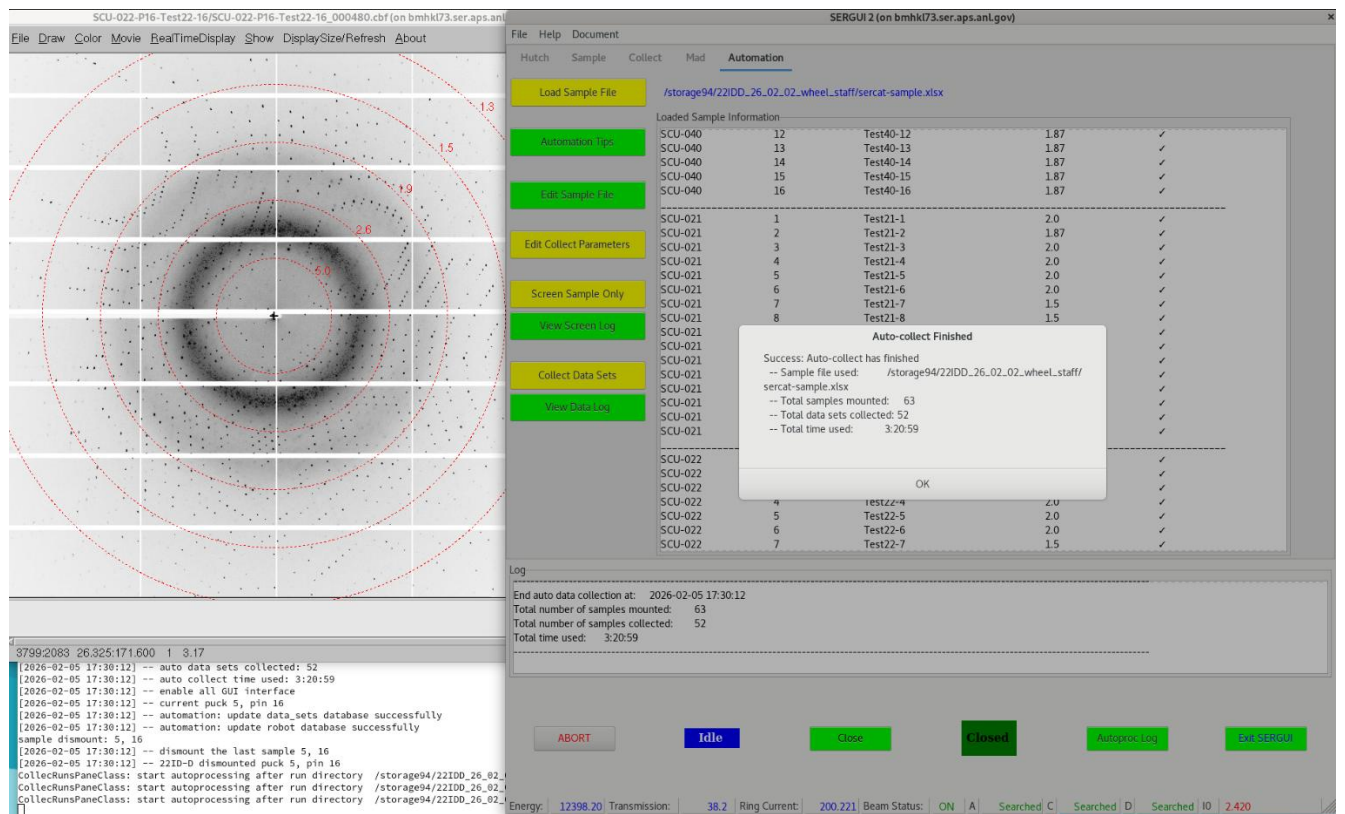
Benchmarking indicates that the automated workflow consistently collects more datasets than manual operation while delivering comparable—or often improved—data quality. The system currently completes one full puck (16 samples) in approximately 50 minutes. By contrast, users typically collect about 10 samples per hour when operating manually. In addition, user fatigue and occasional errors in sample alignment or data-collection setup can compromise data quality, further highlighting the advantages of automation.

These upgrades substantially improve beamline efficiency, throughput, and overall data quality for SER-CAT users. Looking ahead, selected night beamtime periods may be designated as automation slots, allowing users to take advantage of fully automated data collection without the need for advance scheduling. This added flexibility will further expand access and streamline high-throughput crystallography at SER-CAT.



Puck	Pin	Sample	Resolution	AutoCollect
SCU-001		1 Test01-1	2	
SCU-001		2 Test01-2	1.87	1
SCU-001		3 Test01-3	2	1
SCU-001		4 Test01-4	2 NO	
SCU-001		5 Test01-5	2	1
SCU-001		6 Test01-6	2	1
SCU-001		7 Test01-7	1.5	1
SCU-001		8 Test01-8	1.5	1
SCU-001		9 Test01-9	1.5	1
SCU-001		10 Test01-10	1.5	1
SCU-001		11 Test01-11	2	1
SCU-001		12 Test01-12	1.87	1
SCU-001		13 Test01-13	1.87	1
SCU-001		14 Test01-14	1.87	1
SCU-001		15 Test01-15	1.87	1
SCU-001		16 Test01-16	1.87	1
SCU-040		1 Test40-1	2	1
SCU-040		2 Test40-2	1.87	1
SCU-040		3 Test40-3	2	1
SCU-040		4 Test40-4	2	1
SCU-040		5 Test40-5	2	1
SCU-040		6 Test40-6	2	1
SCU-040		7 Test40-7	1.5	1
SCU-040		8 Test40-8	1.5	1
SCU-040		9 Test40-9	1.5	1
SCU-040		10 Test40-10	1.5	1
SCU-040		11 Test40-11	2	1
SCU-040		12 Test40-12	1.87	1
SCU-040		13 Test40-13	1.87	1
SCU-040		14 Test40-14	1.87	1
SCU-040		15 Test40-15	1.87	1
SCU-040		16 Test40-16	1.87	1
SCU-021		1 Test21-1	2	1
SCU-021		2 Test21-2	1.87	1
SCU-021		3 Test21-3	2	1
SCU-021		4 Test21-4	2	1
SCU-021		5 Test21-5	2	1
SCU-021		6 Test21-6	2	1
SCU-021		7 Test21-7	1.5	1
SCU-021		8 Test21-8	1.5	1
SCU-021		9 Test21-9	1.5	1
SCU-021		10 Test21-10	1.5	1
SCU-021		11 Test21-11	2	1
SCU-021		12 Test21-12	1.87	1
SCU-021		13 Test21-13	1.87	1
SCU-021		14 Test21-14	1.87	1
SCU-021		15 Test21-15	1.87	1
SCU-021		16 Test21-16	1.87	1
SCU-022		1 Test22-1	2	1
SCU-022		2 Test22-2	1.87	1
SCU-022		3 Test22-3	2	1
SCU-022		4 Test22-4	2	1
SCU-022		5 Test22-5	2	1
SCU-022		6 Test22-6	2	1
SCU-022		7 Test22-7	1.5	1
SCU-022		8 Test22-8	1.5	1
SCU-022		9 Test22-9	1.5	1
SCU-022		10 Test22-10	1.5	1
SCU-022		11 Test22-11	2	1
SCU-022		12 Test22-12	1.87	1
SCU-022		13 Test22-13	1.87	1
SCU-022		14 Test22-14	1.87	1
SCU-022		15 Test22-15	1.87	1
SCU-022		16 Test22-16	1.87	1

Sample File: sercat_sample.xlsx



Automation finished

Comparison between automated and manual data collection

Manual collection by user														
Reso	Rmerg(low high)	Rdn	Comp	I/sigI-high	ccl/2	Mos	UnitCell				Symm	Location		
dir: /storage94/22IDD_26 {0.5/0.1/368.0/ 1 7671,}														
2.18	0.098(0.058 1.395)	6.7	85.9	10.7	1.0	0.374	0.17	49.50	121.17	88.24	90.00	103.07	90.00	P1211 zzCmdxds_plp2_000001/xs/zzpac_sum.log
2.48	0.127(0.077 0.545)	6.5	61.1	6.5	0.9	0.843	3.16	49.41	120.97	88.03	90.00	103.05	90.00	P21 zzCmddials_plp2_000001/zzCmddials_sum.log
2.27	0.053(0.036 0.372)	3.4	81.8	6.5	1.8	0.267	0.70	48.99	121.21	88.53	90.00	102.34	90.00	P21 zzKylin_plp2_000001/*sum.log
Automated data collection														
Reso	Rmerg(low high)	Rdn	Comp	I/sigI-high	ccl/2	Mos	UnitCell				Symm	Location		
dir: /storage94/22IDD_26 {0.25/0.05/165.0/ 1 19524, 1 22932,}														
2.13	0.071(0.034 1.088)	3.8	98.6	9.3	1.2	0.347	0.20	49.47	121.02	88.14	90.00	103.01	90.00	P1211 zzCmdxds_GT01-P2-GT01_Pin2_000001/xs/zzpac_sum.log
2.08	0.497(0.109 1.051)	3.7	70.8	0.9	0.4	0.307	1.08	49.63	121.46	172.75	90.00	93.30	90.00	P21 zzCmddials_GT01-P2-GT01_Pin2_000001/zzCmddials_sum.log
1.38	0.202(0.081 0.206)	4.2	76.0	3.2	2.1	0.434	0.35	49.64	689.60	121.69	90.00	90.00	90.00	C2221 zzKylin_GT01-P2-GT01_Pin2_000001/*sum.log
Manual collection:														
dir: /storage94/22IDD_26 {0.25/0.15/336.0/ 1 25072,}														
2.99	0.410(0.340 0.610)	3.5	98.4	1.6	0.9	0.688	0.42	48.72	90.24	119.95	90.00	90.00	100.93	P1 zzCmdxds_plp3_000001/xs/zzpac_sum.log
2.41	0.148(0.087 0.610)	5.8	68.4	4.6	0.8	0.833	1.29	49.26	120.85	87.92	90.00	103.00	90.00	P21 zzCmddials_plp3_000001/zzCmddials_sum.log
2.16	0.082(0.058 0.725)	4.4	92.8	9.3	2.1	0.183	0.49	49.51	120.97	91.73	90.00	108.98	90.00	P2 zzKylin_plp3_000001/*sum.log
Automated collection:														
dir: GT01-P3-GT01_Pin3/ {0.25/0.05/165.0/ 1 5910, 1 6053,}														
2.13	0.085(0.037 1.437)	3.7	98.9	8.3	0.9	0.302	0.24	49.58	121.48	88.64	90.00	103.07	90.00	P1211 zzCmdxds_GT01-P3-GT01_Pin3_000001/xs/zzpac_sum.log
2.08	0.297(0.077 0.814)	3.4	76.5	1.6	0.6	0.460	0.67	49.65	121.60	88.70	90.00	103.10	90.00	P21 zzCmddials_GT01-P3-GT01_Pin3_000001/zzCmddials_sum.log
1.44	0.056(0.040 0.351)	2.0	75.3	4.0	1.8	0.193	0.26	48.74	120.89	90.74	90.00	110.34	90.00	P21 zzKylin_GT01-P3-GT01_Pin3_000001/*sum.log

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File	Edit	View	Search	Terminal	Help										

Auto:	dir: /storage94/22IDD_26_02_18_wheel_staff/auto_collect/										{0.25/0.05/185.6/ 1 40524, 1 44758,}				
1.35	0.048(0.033 1.000)	9.6	100.0	19.5	1.0	0.478	0.22	42.51	42.51	79.86	90.00	90.00	120.00	P3121	zzCmdxds_UNC-0059-P2-NA_000001/xs/zzpac_sum.log
1.47	0.060(0.042 0.435)	8.1	87.5	9.3	1.0	0.878	0.79	42.49	42.49	79.83	90.00	90.00	120.00	P3121	zzCmddials_UNC-0059-P2-NA_000001/zzCmddials_sum.log
1.38	0.052(0.043 0.347)	7.2	95.8	19.6	1.9	0.641	0.45	42.34	42.34	79.65	90.00	90.00	120.00	P3121	zzKylin_UNC-0059-P2-NA_000001/*sum.log
Manual:	dir: /storage94/22IDD_26_02_18_wheel_staff/auto_collect/										{0.25/0.05/203.0/ 1 4232, 1 9090,}				
1.47	0.069(0.041 1.341)	9.8	100.0	15.2	0.9	0.419	0.20	42.83	42.83	80.46	90.00	90.00	120.00	P3121	zzCmdxds_closer_p4p2_000001/xs/zzpac_sum.log
1.65	0.083(0.052 0.450)	8.0	86.7	6.2	1.0	0.875	0.88	42.32	42.32	79.48	90.00	90.00	120.00	P3121	zzCmddials_closer_p4p2_000001/zzCmddials_sum.log
1.49	0.052(0.042 0.445)	7.1	97.9	12.4	1.9	0.072	0.33	42.74	42.74	80.02	90.00	90.00	120.00	P3121	zzKylin_closer_p4p2_000001/*sum.log
Note: Auto yielded higher resolution & I/Sig(I) and better R-merg [over all comparable]															

Auto:	dir: /storage94/22IDD_26_02_18_wheel_staff/auto_collect/										{0.25/0.1/185.6/ 1 3281, 1 986,}				
1.46	0.069(0.044 0.397)	3.9	87.7	4.0	2.3	0.219	0.38	36.01	41.01	114.03	90.00	90.00	90.00	P212121	zzKylin_UNC-0059-P3-NA_000001/*sum.log
1.92	0.180(0.150 2.458)	6.8	99.4	6.3	0.9	0.345	0.49	35.61	40.62	112.65	90.00	90.00	90.00	P22121	zzCmdxds_UNC-0059-P3-NA_000001/xs/zzpac_sum.log
Manual:	dir: /storage94/22IDD_26_02_18_wheel_staff/auto_collect/										{0.25/0.05/271.0/ 1 17515,}				
1.92	0.057(0.041 0.407)	2.2	68.7	4.6	1.6	0.202	0.67	35.78	41.08	113.70	90.00	90.00	90.00	P22121	zzKylin_closer_p4p3_000001/*sum.log
Note: Auto yielded higher I/Sig(I) and better completeness [over all comparable]															

Auto:	dir: /storage94/22IDD_26_02_18_wheel_staff/auto_collect/										{0.25/0.05/185.6/ 1 21771, 1 25140,}				
1.49	0.043(0.035 0.775)	2.6	82.8	6.3	1.7	0.188	0.86	62.41	67.07	66.44	90.00	111.56	90.00	C2	zzKylin_UNC-0059-P5-NA_000001/*sum.log
Manual:	dir: /storage94/22IDD_26_02_18_wheel_staff/auto_collect/										{0.25/0.05/203.0/ 1 11335,}				
2.15	0.161(0.109 1.111)	3.3	93.4	4.4	1.3	0.342	0.42	61.39	67.27	66.62	90.00	113.17	90.00	C121	zzCmdxds_closer_p4p5_000001/xs/zzpac_sum.log
1.83	0.118(0.047 0.647)	3.3	69.0	3.9	0.5	0.597	2.28	60.87	66.74	65.98	90.00	113.07	90.00	C121	zzCmddials_closer_p4p5_000001/zzCmddials_sum.log
1.45	0.055(0.029 0.264)	3.0	77.9	2.9	1.8	0.566	2.70	60.37	67.00	65.19	90.00	111.85	90.00	C2	zzKylin_closer_p4p5_000001/*sum.log
Note: Auto yielded better R-merg, but other values little better in manual [over all comparable]															

Auto:	dir: /storage94/22IDD_26_02_18_wheel_staff/auto_collect/										{0.25/0.05/185.6/ 1 19113, 1 17366,}				
2.49	0.246(0.111 1.114)	7.5	99.9	2.7	0.9	0.769	0.19	82.89	82.89	189.35	90.00	90.00	90.00	P212121	zzCmdxds_UNC-0059-P8-NA_000001/xs/zzpac_sum.log
2.51	0.531(0.130 0.481)	6.0	82.3	0.5	0.7	0.932	1.03	82.92	82.92	189.42	90.00	90.00	90.00	P212121	zzCmddials_UNC-0059-P8-NA_000001/zzCmddials_sum.log
1.98	0.047(0.018 0.299)	5.6	94.6	4.3	2.7	0.083	0.21	82.34	82.34	188.80	90.00	90.00	90.00	P42212	zzKylin_UNC-0059-P8-NA_000001/*sum.log
Manual:	dir: /storage94/22IDD_26_02_18_wheel_staff/auto_collect/										{0.25/0.05/229.0/ 1 33710,}				
2.08	0.284(0.144 0.706)	11.2	82.6	1.3	0.6	0.899	0.53	82.89	82.89	189.40	90.00	90.00	90.00	P42212	zzCmddials_closer_p4p8_000001/zzCmddials_sum.log
1.60	0.048(0.030 0.216)	4.7	90.1	6.4	2.1	0.877	0.23	82.85	82.85	188.93	90.00	90.00	90.00	P41212	zzKylin_closer_p4p8_000001/*sum.log
1.93	0.196(0.095 5.000)	13.9	99.9	8.2	0.6	0.498	0.12	82.89	82.89	189.41	90.00	90.00	90.00	P42212	zzCmdxds_closer_p4p8_000001/xs/zzpac_sum.log
Note: Auto yielded better R-merg & I/Sig(I) [over all comparable]															

□

(Note: partial data sets collected in some cases for quick tests)

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File	Ed	View	Search	Terminal	Help											
1.27 0.109(0.036 0.914)	4.0	76.0	12.0	1.7	0.196	0.33	54.31	58.25	66.44	90.00	90.00	90.00	90.00	P22121	zzCmddials	SCU-022-P1-Test22-1.000001/zzCmddials_sum.log
1.29 0.044(0.032 0.414)	2.5	68.9	7.7	1.6	0.138	0.23	54.27	58.17	66.52	90.00	90.00	90.00	90.00	P22122	zzKylin	SCU-022-P1-Test22-1.000001/sum.log
dir: /storage94/22100.26.02.02_wheel_staff/auto_collect/SCU-022-P2-Test22-2/ (0.25/0.05/165.0/ 1 13357, 1 11342.)																
1.12 0.039(0.031 0.357)	3.9	76.2	19.5	2.5	0.466	0.09	54.33	58.27	66.47	90.00	90.00	90.00	90.00	P22122	zzCmddxs	SCU-022-P2-Test22-2.000001/xs/zzpac_sum.log
1.10 0.050(0.044 0.172)	3.9	76.9	25.2	4.0	0.915	0.25	54.32	58.26	66.41	90.00	90.00	90.00	90.00	P22122	zzCmddials	SCU-022-P2-Test22-2.000001/zzCmddials_sum.log
1.30 0.051(0.044 0.123)	3.8	93.7	19.6	8.2	0.895	0.23	54.45	58.40	66.66	90.00	90.00	90.00	90.00	P22122	zzKylin	SCU-022-P2-Test22-2.000001/sum.log
dir: /storage94/22100.26.02.02_wheel_staff/auto_collect/SCU-022-P3-Test22-3/ (0.25/0.05/165.0/ 1 42546, 1 40911.)																
1.12 0.027(0.022 0.108)	3.8	79.1	23.8	3.3	0.964	0.11	54.48	58.20	66.48	90.00	90.00	90.00	90.00	P22121	zzCmddxs	SCU-022-P3-Test22-3.000001/xs/zzpac_sum.log
1.12 0.038(0.031 0.213)	3.8	79.4	24.1	2.9	1.36	0.17	54.47	58.22	66.44	90.00	90.00	90.00	90.00	P22121	zzCmddials	SCU-022-P3-Test22-3.000001/zzCmddials_sum.log
1.30 0.041(0.031 0.151)	4.0	96.8	20.6	7.4	0.943	0.21	54.31	58.15	66.36	90.00	90.00	90.00	90.00	P22121	zzKylin	SCU-022-P3-Test22-3.000001/sum.log
dir: /storage94/22100.26.02.02_wheel_staff/auto_collect/SCU-022-P4-Test22-4/ (0.25/0.05/165.0/ 1 42619, 1 80391.)																
1.12 0.026(0.025 0.114)	3.7	81.8	28.3	7.2	0.472	0.09	54.39	58.24	66.37	90.00	90.00	90.00	90.00	P22121	zzCmddxs	SCU-022-P4-Test22-4.000001/xs/zzpac_sum.log
1.10 0.037(0.038 0.069)	3.7	81.7	28.9	6.7	0.994	0.28	54.40	58.26	66.38	90.00	90.00	90.00	90.00	P22121	zzCmddials	SCU-022-P4-Test22-4.000001/zzCmddials_sum.log
1.30 0.053(0.045 0.116)	4.0	95.0	28.1	9.3	0.919	0.22	54.38	58.29	66.31	90.00	90.00	90.00	90.00	P22122	zzKylin	SCU-022-P4-Test22-4.000001/sum.log
dir: /storage94/22100.26.02.02_wheel_staff/auto_collect/SCU-022-P5-Test22-5/ (0.25/0.05/165.0/ 1 32280, 1 37696.)																
1.12 0.039(0.040 0.430)	3.6	83.9	17.5	1.8	0.843	0.08	54.42	58.24	66.53	90.00	90.00	90.00	90.00	P22121	zzCmddxs	SCU-022-P5-Test22-5.000001/xs/zzpac_sum.log
1.12 0.041(0.034 0.410)	3.6	83.8	22.0	2.5	0.077	0.23	54.36	58.19	66.46	90.00	90.00	90.00	90.00	P22121	zzCmddials	SCU-022-P5-Test22-5.000001/zzCmddials_sum.log
1.30 0.044(0.035 0.172)	3.8	96.3	15.8	3.8	0.885	0.31	54.34	58.16	66.29	90.00	90.00	90.00	90.00	P22121	zzKylin	SCU-022-P5-Test22-5.000001/sum.log
dir: /storage94/22100.26.02.02_wheel_staff/auto_collect/SCU-022-P6-Test22-6/ (0.25/0.05/165.0/ 1 18617, 1 25573.)																
1.12 0.057(0.032 0.721)	3.9	76.4	12.0	0.7	0.136	0.10	54.28	58.19	66.66	90.00	90.00	90.00	90.00	P22121	zzCmddxs	SCU-022-P6-Test22-6.000001/xs/zzpac_sum.log
1.10 0.060(0.038 0.410)	3.9	76.8	14.9	1.0	0.466	0.30	54.22	58.13	65.99	90.00	90.00	90.00	90.00	P22122	zzCmddials	SCU-022-P6-Test22-6.000001/zzCmddials_sum.log
1.29 0.037(0.030 0.191)	3.6	82.8	18.5	5.4	0.446	0.17	54.19	57.97	66.34	90.00	90.00	90.00	90.00	P22121	zzKylin	SCU-022-P6-Test22-6.000001/sum.log
dir: /storage94/22100.26.02.02_wheel_staff/auto_collect/SCU-022-P7-Test22-7/ (0.25/0.05/165.0/ 1 54374, 1 55041.)																
1.12 0.028(0.027 0.095)	4.0	75.3	27.7	5.8	0.279	0.07	54.40	58.23	66.41	90.00	90.00	90.00	90.00	P222	zzCmddxs	SCU-022-P7-Test22-7.000001/xs/zzpac_sum.log
1.12 0.038(0.041 0.252)	4.0	75.1	40.3	13.6	0.049	0.12	54.38	58.21	66.39	90.00	90.00	90.00	90.00	P2212	zzCmddials	SCU-022-P7-Test22-7.000001/zzCmddials_sum.log
1.30 0.024(0.017 0.117)	4.0	92.1	16.1	8.3	0.920	0.16	54.40	58.26	66.42	90.00	90.00	90.00	90.00	P222	zzKylin	SCU-022-P7-Test22-7.000001/sum.log
dir: /storage94/22100.26.02.02_wheel_staff/auto_collect/SCU-022-P8-Test22-8/ (0.25/0.05/165.0/ 1 43332, 1 43514.)																
1.12 0.034(0.030 0.545)	3.9	76.4	24.6	1.8	0.589	0.12	54.30	58.27	66.48	90.00	90.00	90.00	90.00	P222	zzCmddxs	SCU-022-P8-Test22-8.000001/xs/zzpac_sum.log
1.12 0.039(0.029 0.454)	3.9	76.1	20.8	1.5	0.024	0.35	54.32	58.29	66.51	90.00	90.00	90.00	90.00	P22121	zzCmddials	SCU-022-P8-Test22-8.000001/zzCmddials_sum.log
1.29 0.034(0.028 0.188)	3.9	93.3	19.6	4.2	0.888	0.31	54.15	58.09	66.25	90.00	90.00	90.00	90.00	P222	zzKylin	SCU-022-P8-Test22-8.000001/sum.log
dir: /storage94/22100.26.02.02_wheel_staff/auto_collect/SCU-022-P9-Test22-9/ (0.25/0.05/165.0/ 1 94559, 1 27624.)																
1.31 0.114(0.042 0.809)	4.1	95.8	13.5	1.5	0.367	0.19	54.20	58.28	66.34	90.00	90.00	90.00	90.00	P222	zzCmddxs	SCU-022-P9-Test22-9.000001/xs/zzpac_sum.log
1.21 0.067(0.054 0.357)	3.9	76.9	9.9	0.9	0.796	0.55	54.31	58.28	66.42	90.00	90.00	90.00	90.00	P2212	zzCmddials	SCU-022-P9-Test22-9.000001/zzCmddials_sum.log
1.30 0.048(0.038 0.311)	3.6	85.6	14.0	2.3	0.641	0.20	54.28	58.30	66.47	90.00	90.00	90.00	90.00	P222	zzKylin	SCU-022-P9-Test22-9.000001/sum.log
dir: /storage94/22100.26.02.02_wheel_staff/auto_collect/SCU-022-P10-Test22-10/ (0.25/0.05/165.0/ 1 71017, 1 50658.)																
1.12 0.031(0.033 0.087)	3.8	77.6	27.7	8.1	0.670	0.06	54.36	58.19	66.47	90.00	90.00	90.00	90.00	P22121	zzCmddxs	SCU-022-P10-Test22-10.000001/xs/zzpac_sum.log
1.10 0.042(0.050 0.146)	3.8	77.7	29.8	7.5	0.607	0.11	54.35	58.18	66.46	90.00	90.00	90.00	90.00	P22121	zzCmddials	SCU-022-P10-Test22-10.000001/zzCmddials_sum.log
1.29 0.051(0.051 0.105)	4.0	95.6	21.7	11.3	0.953	0.16	54.32	58.10	66.32	90.00	90.00	90.00	90.00	P22121	zzKylin	SCU-022-P10-Test22-10.000001/sum.log
dir: /storage94/22100.26.02.02_wheel_staff/auto_collect/SCU-022-P11-Test22-11/ (0.25/0.05/165.0/ 1 41963, 1 45242.)																
1.12 0.024(0.025 0.085)	3.7	80.2	31.8	7.7	0.526	0.07	54.38	58.22	66.48	90.00	90.00	90.00	90.00	P22121	zzCmddxs	SCU-022-P11-Test22-11.000001/xs/zzpac_sum.log
1.10 0.033(0.039 0.232)	3.8	84.4	36.0	8.3	0.211	0.13	54.36	58.21	66.46	90.00	90.00	90.00	90.00	P22121	zzCmddials	SCU-022-P11-Test22-11.000001/zzCmddials_sum.log
1.30 0.044(0.040 0.108)	4.1	97.2	23.9	11.7	0.971	0.17	54.33	58.06	66.40	90.00	90.00	90.00	90.00	P22121	zzKylin	SCU-022-P11-Test22-11.000001/sum.log
dir: /storage94/22100.26.02.02_wheel_staff/auto_collect/SCU-022-P12-Test22-12/ (0.25/0.05/165.0/ 1 34929, 1 73823.)																
1.12 0.038(0.037 0.148)	3.7	82.1	24.8	3.5	0.984	0.07	54.40	58.21	66.54	90.00	90.00	90.00	90.00	P222	zzCmddxs	SCU-022-P12-Test22-12.000001/xs/zzpac_sum.log
1.12 0.036(0.027 0.236)	3.7	81.7	27.3	4.3	0.028	0.13	54.35	58.17	66.49	90.00	90.00	90.00	90.00	P22122	zzCmddials	SCU-022-P12-Test22-12.000001/zzCmddials_sum.log
1.30 0.038(0.029 0.142)	4.1	93.5	19.9	5.5	0.965	0.16	54.39	58.26	66.53	90.00	90.00	90.00	90.00	P222	zzKylin	SCU-022-P12-Test22-12.000001/sum.log
dir: /storage94/22100.26.02.02_wheel_staff/auto_collect/SCU-022-P13-Test22-13/ (0.25/0.05/165.0/ 1 44267, 1 96482.)																
1.12 0.022(0.020 0.068)	3.7	81.0	33.7	8.2	0.726	0.06	54.39	58.22	66.36	90.00	90.00	90.00	90.00	P22121	zzCmddxs	SCU-022-P13-Test22-13.000001/xs/zzpac_sum.log
1.12 0.031(0.033 0.144)	3.8	81.1	35.2	9.4	0.229	0.10	54.39	58.24	66.38	90.00	90.00	90.00	90.00	P22121	zzCmddials	SCU-022-P13-Test22-13.000001/zzCmddials_sum.log
1.30 0.034(0.032 0.095)	4.1	97.0	27.6	10.7	0.973	0.16	54.38	58.24	66.41	90.00	90.00	90.00	90.00	P222	zzKylin	SCU-022-P13-Test22-13.000001/sum.log
dir: /storage94/22100.26.02.02_wheel_staff/auto_collect/SCU-022-P14-Test22-14/ (0.25/0.05/165.0/ 1 33651, 1 85638.)																
1.11 0.032(0.030 0.164)	4.3	69.9	25.5	5.3	0.925	0.06	54.43	58.21	66.53	90.00	90.00	90.00	90.00	P222	zzCmddxs	SCU-022-P14-Test22-14.000001/xs/zzpac_sum.log
1.10 0.041(0.039 0.116)	4.4	69.7	34.7	7.3	0.962	0.11	54.41	58.20	66.52	90.00	90.00	90.00	90.00	P22122	zzCmddials	SCU-022-P14-Test22-14.000001/zzCmddials_sum.log
1.30 0.038(0.037 0.096)	4.4	87.6	23.1	9.2	0.969	0.14	54.44	58.23	66.52	90.00	90.00	90.00	90.00	P222	zzKylin	SCU-022-P14-Test22-14.000001/sum.log
dir: /storage94/22100.26.02.02_wheel_staff/auto_collect/SCU-022-P15-Test22-15/ (0.25/0.05/165.0/ 1 51968, 1 85257.)																
1.11 0.035(0.032 0.304)	3.6	81.6	16.8	1.1	0.523	0.14	54.18	58.24	66.43	90.00	90.00	90.00	90.00	P22121	zzCmddxs	SCU-022-P15-Test22-15.000001/xs/zzpac_sum.log
1.10 0.044(0.030 0.448)	3.6	82.4	19.3	1.3	0.037	0.41	54.29	58.41	66.63	90.00	90.00	90.00	90.00	P22121	zzCmddials	SCU-022-P15-Test22-15.000001/zzCmddials_sum.log
1.30 0.046(0.034 0.165)	3.8	96.6	18.4	5.8	0.884	0.28	54.36	58.29	66.55	90.00	90.00	90.00	90.00	P22121	zzKylin	SCU-022-P15-Test22-15.000001/sum.log
dir: /storage94/22100.26.02.02_wheel_staff/auto_collect/SCU-022-P16-Test22-16/ (0.25/0.05/165.0/ 1 54617, 1 53694.)																
1.12 0.022(0.020 0.125)	3.7	79.6	33.4	5.6	0.952	0.09	54.38	58.24	66.64	90.00	90.00	90.00	90.00	P222	zzCmddxs	SCU-022-P16-Test22-16.000001/xs/zzpac_sum.log
1.10 0.037(0.039 0.151)	3.8	79.0	30.2	5.7	0.959	0.24	54.39	58.25	66.64	90.00	90.00	90.00	90.00	P22121	zzCmddials	SCU-022-P16-Test22-16.000001/zzCmddials_sum.log
1.30 0.061(0.051 0.173)	4.0	94.3	19.3	9.5	0.818	0.34	54.42	58.28	66.68	90.00	90.00	90.00	90.00	P222	zzKylin	SCU-022-P16-Test22-16.000001/sum.log
nTotalDataDirSearched=75 nResultsFound=275 processed by axdpro parallel																

Automation tips:

When setting up the automated data collection through “Automation” tab on SERGUI:

** Load Sample file **

- spread sheet .xlsx file format is needed
- must have five columns with labels beginning with "Puck" "Pin" "Sample" "Resolution" "AutoCollect"
- extra columns with different labels are allowed for users own note
- "Puck" names should match with SERGUI loaded "Puck List"
- if they don't match, you may ask staff to change loaded pucks' names or edit and reload your own sample file
- there should NOT be any special characters and spaces in your Puck names and Sample names
- "-" and "_" characters are allowed
- "Pin" must be number between 1-16 in the puck positions
- "AutoCollect" column for each sample will mark the sample to be auto-collected
 - empty space will bypass the sample in autocollect process
 - any non-empty characters or words would mark the sample for data collection
- if you don't have a .xlsx file ready to load, you may download a template file from SERGUI
 - SERGUI -> Document -> Download SER-CAT Sample Template File
 - sercat-sample.xlsx file will be saved in your main data directory
 - edit the downloaded file and reload it
- "Load Sample" file when you have file ready to load

** Edit Sample File **

- click this button, if you need to edit your loaded sample file

-- after editing, save the file, exit the file editor, program will automatically "Load Sample" again

**** Edit Collect Parameters ****

-- "Scan Width", "Exposure Time", "Transmission", "Degree Range" will be used for all samples in automation

-- "Resolution" can be empty or given a value

-- if empty:

-- Autoscreen will move detector distance to 200 mm (1.5 Å) for all screening

-- Autocollect will use "Resolution" values provided in loaded Sample File for each sample data collections

-- if given a value:

-- Autoscreen will use this given resolution value to override any sample file values for all screenings

-- Autocollect will use this given resolution values to override any sample file values for all data collections

**** Option 1: Screen Sample Only ****

-- this autoscreen routine will go through every sample in the loaded Sample File

-- routine: mount sample -> auto loop centering -> 2D raster -> collect single -> autoindex

-- result will be saved in log file, as example "sercat-sample_autoscreen_2025-11-29.log"

**** Option 2: Collect Data Sets ****

-- this autocollect routine will collect sample marked in "AutoCollect" column

-- routine: mount sample -> auto loop centering -> 3D raster -> single image index screen
-> collect data set -> autoprocess

-- result will be saved in log file, as example "sercat-sample_autocollect_2025-11-29.log"

***** Important Notice *****

- please don't interact with sergui during autoscreen or autocollect
- automation status will be updated on the screen during automation
- after automation is finished, the GUI will be enabled
- "View Screen Log" or "View Data Log" to check results
- currently, autoscreen will take about 1 minute for each sample
- currently, autocollect will take about 2-3 minutes for each sample with default data collection parameters