

FAIR data at the NIST Center for Neutron Research

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NCNR: a neutron-beam user facility

*"a national resource for
industry, universities, and
government agencies."*

22 Scattering Instruments

(8 additional Physics/Analytical Chemistry)

- Crystallography
- Reflectometry
- Small-Angle Neutron Scattering (SANS)
- Spectroscopy

<https://www.nist.gov/ncnr>

NCNR user program (per year*)

774 beamtime proposals

2769 users

Institutions:

- 17 NIST Divisions and Offices
- 38 U.S. Government Laboratories
- 42 U.S. States + DC + Puerto Rico
- 50 U.S. Corporations
- 181 U.S. Universities

CHRNS: Center for High Resolution Neutron Scattering (NSF)

- Instruments (266 proposals in 2019):
 1. [CHRNS Very Small Angle Neutron Scattering \(vSANS\)](#)
 2. [CHRNS Multi-Axis Crystal Spectrometer \(MACS\)](#)
 3. [CHRNS High-Flux Backscattering Spectrometer \(HFBS\)](#)
 4. [CHRNS Neutron Spin Echo Spectrometer \(NSE\)](#)
 5. [CHRNS White Beam Reflectometer \(CANDOR\)](#)
- Support for NCNR proposal system
- Non-Equilibrium Science initiative
- FAIR data initiative (beginning FY2021)



Raw data:
open by
default

- Oldest: [NG3SANS \(1989-02-08\)](#)
- Total number: 4,425,906 files
- Total size: 1.2 TB
- DOI: <https://dx.doi.org/10.18434/T4201B>
 - Points to: <https://ncnr.nist.gov/pub/ncnrdata/>

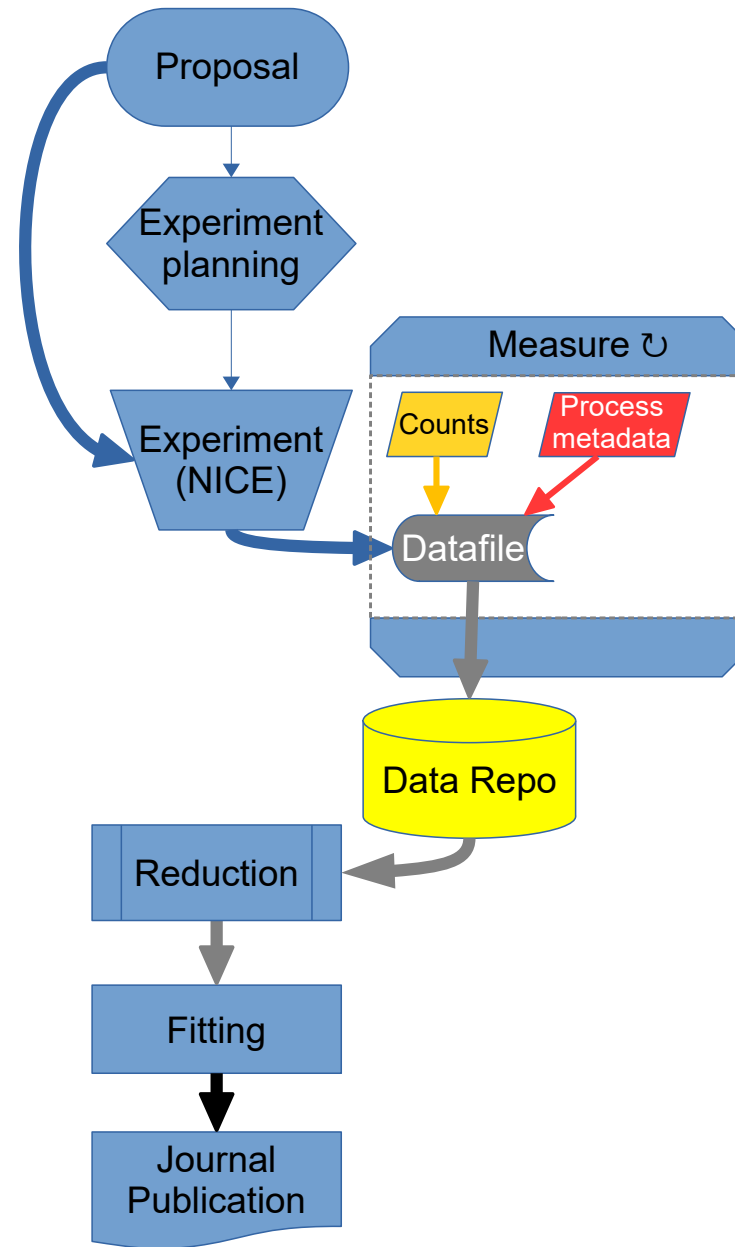
NCNR Data Management Plan:

All NCNR raw data within the scope stated above are made available to the public following an experiment unless the researcher ... opts out ...

NCNR and FAIR data: up to 2020

- [Open raw data](#)
- [Limited search by metadata](#) (file date, name, description)
- [Live instrument data display](#) since 2008
- [Online data reduction](#): 2017 (reflectometry)
- Custom web-based data viewers
 - [Column-format](#) (text)
 - [NeXus](#) (HDF5)

Data and Metadata Lifecycle (before)



CHRNS (NSF)
FAIR data
sprint

During unplanned reactor
outage of 2021



Accelerate FAIR initiatives

ORCID
integration

DOI per
experiment

search data
by metadata

capture of
process
metadata

traceable
data
reduction
workflows

ORCiD integration

Proposal system:

- Federated login
- User disambiguation

Instrument Control:

- ORCiDs pulled from proposal
- Re-transmitted to data.nist.gov

Experiment DOI record in data.nist.gov

Future:

- User identity management for remote computing

FAIR sprint contributors

Instrument control software team

- *Steve Pheiffer, Nick Siebenlist, Natasha Shmunis, Chirag Parikh, Fawaz Joseph*
- Sample metadata taxonomy and management
- Initiating DOI creation on new experiments
- Capturing process metadata

NCNR center office

- *Siddharth Khosla, Alan Munter*
- Integration of ORCID identity management across facility

Scientific staff

- *Tyler Martin, Katie Weigandt, William Ratcliff...*
- Development of taxonomies
- Identifying incentives
- Curating process metadata

Citeable data: DOI per experiment



Through NIST Science Data Portal <https://data.nist.gov>



Automated pre-publish through API on experiment start



Metadata populated from proposal:

Participants, including ORCID

Title, Description

Activity dates/times

Links to raw data DOI, search functions, etc.

Searchable metadata

Define metadata for sample

Flexible JSON record with unique ID

Sample associated with measurement

Associations published with data

Document database from records

Public search API

Human-friendly search tools

UUID	Local ID	Name	Description	volume_fraction	magnetic_field	geometry
a35edece-15ae-41e0-8e81-dbf7a78b5e8b	9					
316aceb4-73cb-488f-be86-c243e0e8876c	10					
6a6afb6a-ef1f-488a-ac55-c839e4e9fa5f	11					

Ensure that workflows in instrument control software include

Measurement intent

- Background
- Transmission
- Scattering ...

Sample environment

- Temperature
- Magnetic Field
- Frequency ...



Capture process metadata

Add process variables to searchable metadata

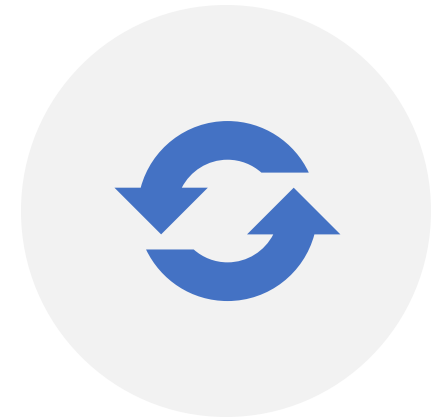
Traceable data workflows



TRACK HISTORY OF
PROCESSING STEPS

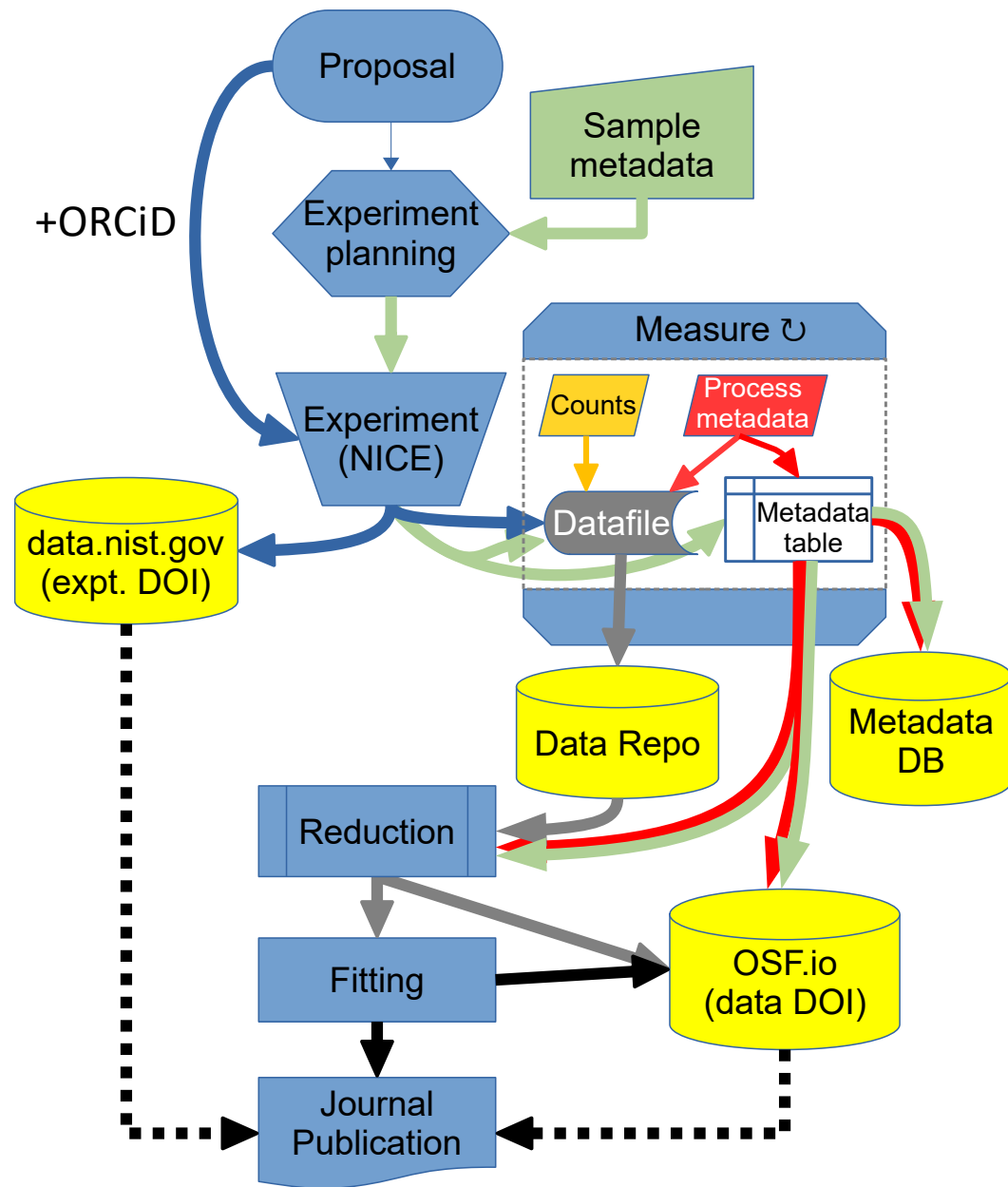


EMBED OR EXPORT
PROCESSING RECIPES

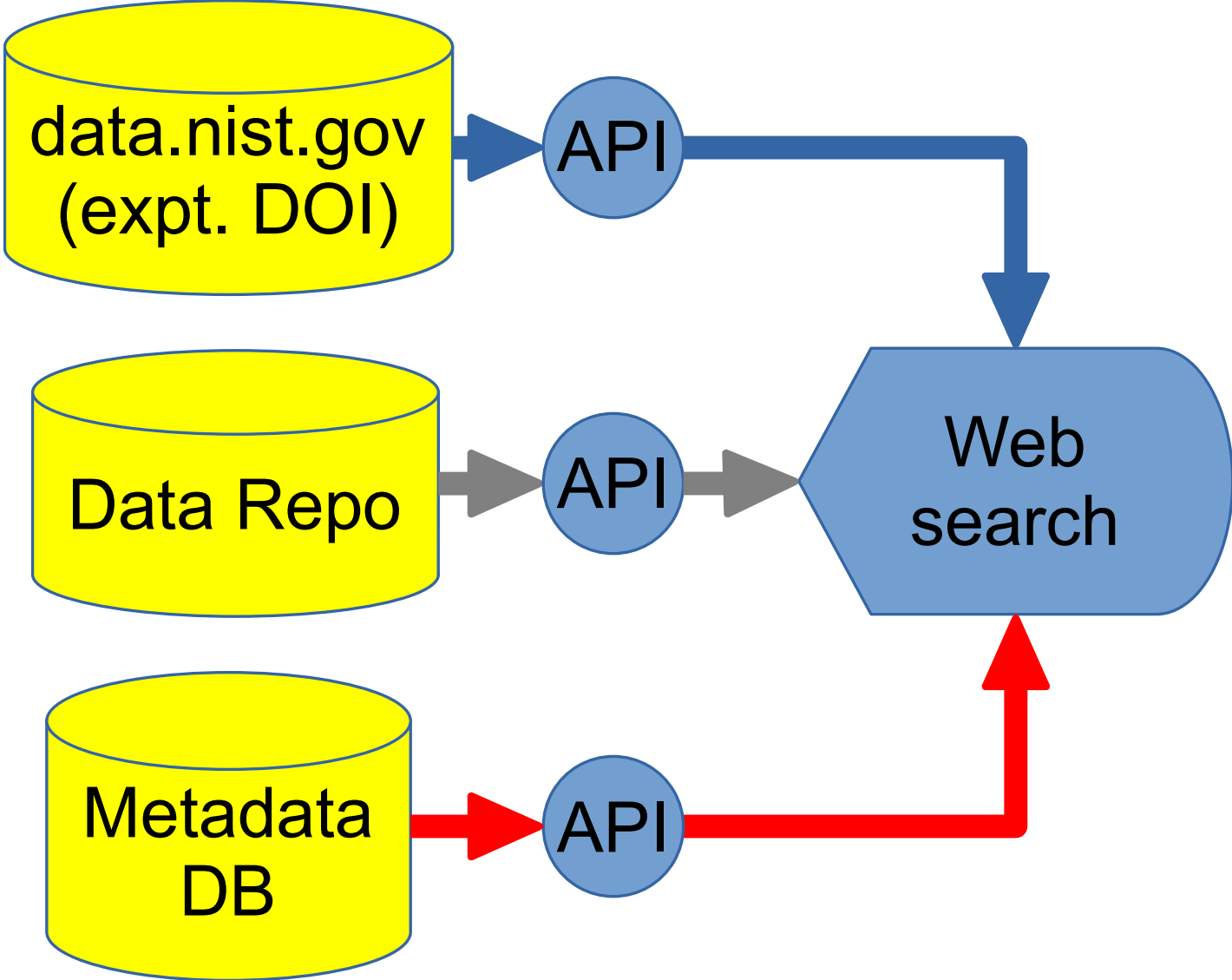


SUPPORT REPLAY

Data and Metadata Lifecycle (after)



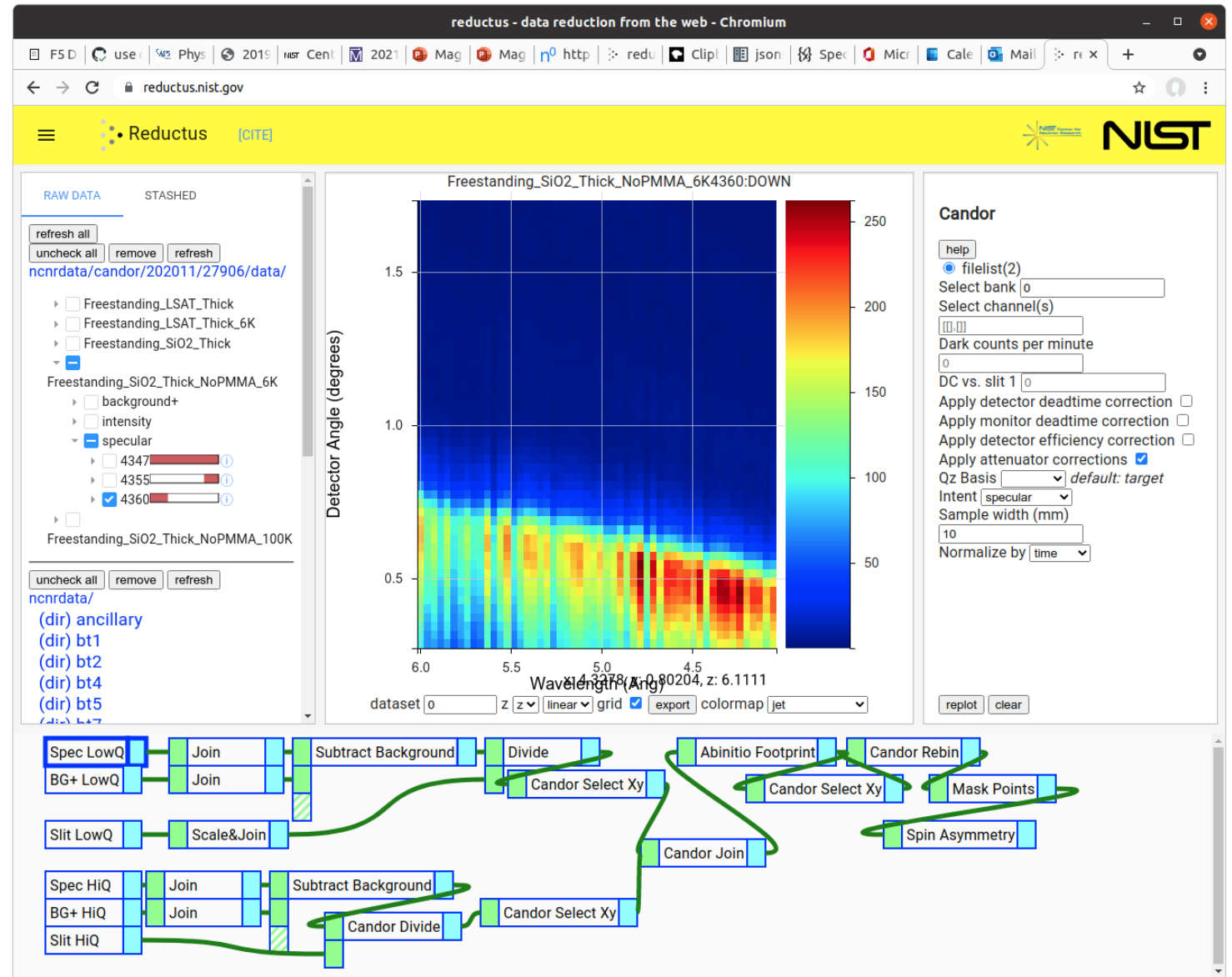
Public data
accessibility



Nice things you can do
with FAIR data...

Online data reduction

- <https://reductus.nist.gov>
- Data accessed directly using data repo and API
- Anonymous, stateless
- Python backend
- Feed-in from other tools e.g. [experiment browser](#)



Upgrades to raw data repository web view

- DOI direct link
- SHA-256 integrity hash
- "Download All" button
- Future: File type (mime)
- Future: Viewer links

Index of /pub/ncnrdata/pbr/202007/27003/data

Name	Last modified	Size	Description
Parent Directory			
SnTe-CBST-SL77317.nxz.ngd	2020-08-03 18:48	386K	
SnTe-CBST-SL77318.nxz.ngd	2020-08-03 21:46	440K	
SnTe-CBST-SL77319.nxz.ngd	2020-08-04 00:04	422K	
SnTe-CBST-SL77376.nxz.ngd	2020-08-04 03:27	389K	
SnTe-CBST-SL77377.nxz.ngd	2020-08-04 06:25	448K	
SnTe-CBST-SL77378.nxz.ngd	2020-08-04 08:44	428K	



NIST Center for Neutron Research Data Repository

DOI: <https://dx.doi.org/10.18434/T4201B?urlappend=magik/202001/26868/data/>

[ncnrdata/](#) [magik/](#) [202001/](#) [26868/](#) [data/](#)

Subdirectories

Name Last Modified

Files

[Download all \(.zip\)](#)

Name	Last Modified ▼	Size	SHA-256
fp_slitAperture4.softPosition25479.nxz.cgd	2020-02-07 19:17:25	169K	336EAA413E5B2B6...
fp_slitAperture4.softPosition_25479.cgd	2020-02-07 19:17:24	976B	79D9711F13A8667...
fp_slitAperture3.softPosition25478.nxz.cgd	2020-02-07 19:16:08	168K	AD4DE71B7F08251...
fp_slitAperture3.softPosition_25478.cgd	2020-02-07 19:16:08	976B	8163EA89DFB4F5D...
fp_slitAperture2.softPosition25477.nxz.cgd	2020-02-07 19:15:00	168K	A56400172DBF0D3...
fp_slitAperture2.softPosition_25477.cgd	2020-02-07 19:15:00	976B	6533BE26676BF21...
fp_slitAperture1.softPosition25476.nxz.cgd	2020-02-07 19:13:49	168K	62BAB5A1306645F...
fp_slitAperture1.softPosition_25476.cgd	2020-02-07 19:13:48	976B	37E61E5AD1E0AA2...
fp_detectorAngle.softPosition25475.nxz.cgd	2020-02-07 19:12:33	169K	7AED22035587A48...
fp_detectorAngle.softPosition_25475.cgd	2020-02-07 19:12:33	2K	4855C612E31FDB8...
fp_slitTrans3.softPosition25474.nxz.cgd	2020-02-07 19:03:25	162K	5B5E6CB1822F319...
fp_slitTrans3.softPosition_25474.cgd	2020-02-07 19:03:25	1K	AE65028C76CAD4D...

Public Data viewers

- [Live data](#) (all instruments)
- [CHRNS VSANS viewer](#)
- [CHRNS CANDOR viewer](#)
- [Column-data viewer](#)
- [NeXus inspector](#)

