



NexusLIMS: Automated Research Data Management in Multi-User Characterization Facilities with NEMO

<https://datasophos.co/nexuslims> 

MIT.nano NEMO User Meeting

Josh Taillon October 5, 2026

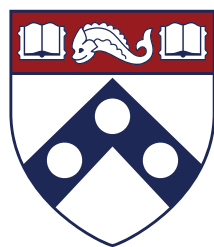
Acknowledgements

Ongoing NexusLIMS support



Jamie Ford

Singh Center for Nanotechnology,
University of Pennsylvania



**Singh Center for
Nanotechnology**
UNIVERSITY of PENNSYLVANIA

Original NexusLIMS Team at NIST



June Lau



Gretchen Greene



Ryan White



and many other colleagues

Established the foundation for today's NexusLIMS.

CDCS project team at NIST

Benjamin Long · Guillaume Sousa Amaral · Philippe Dessauw

For the [CDCS platform](#) behind the NexusLIMS frontend.

About Me



Josh Taillon

Ph.D. in Materials Science & Engineering, Univ. of Maryland (2016)

Analytical electron microscopy; open-source spectral data analysis
TEM, SEM, EELS, EDS, FIB/SEM, etc.

2016 to 2025 – NIST Office of Data and Informatics

Built the NexusLIMS data management system; community consensus-building on metadata standards for materials; data workflows for various materials research domains

Since 2025 – Industry and Entrepreneurship

Principal Software Engineer @ [Posit, PBC](#) – Building open-source tools for AI and data science
Founded **datasophos, LLC** – unexpectedly an entrepreneur!

ABOUT DATASOPHOS

datasophos, LLC helps research organizations navigate the open source landscape and builds custom solutions for their unique needs.

 datasophos.co

 joshuataillon.com

 josh@datasophos.co

The Motivation: A Dark Data Iceberg

We collect far more data than we publish.

- Published results and repositories capture only a fraction of what we acquire
- “Available upon request” (*right...*) leaves much of the data hard to find and reuse
- Sample history, instrument conditions, notes, and negative results are often left behind

Without context, data loses much of its value.

Visible Data

Dark Data

Published Results

Curated records, figures, published images, conclusions, etc. Just a tiny fraction of what was acquired.

Data Repositories

Some institutions or funders enforce data publication requirements. This is better than nothing, but often not the whole story.

Project Context

User proposals, experimental goals, hypotheses, information from previous experiments... the “why”

Sample Provenance

What is it, where did it come from, how was it prepared, history of treatment

Experimental Setup

Instrument conditions, calibration information, tool status, reservation context, environmental conditions, etc.

Negative Results

Dead ends and “bad data” are often collected, looked at once, and either deleted or completely forgotten about. Even “bad” data can have value with the right context!

Human Feedback

Notes during experiments, feedback from analysis and collaborators, linkages to derived datasets

What is NexusLIMS?

It is an open-source **laboratory information management system** (LIMS) for materials characterization facilities — originally developed while I was at NIST, now maintained as an open-source community project by **datasophos, LLC**.

Key features:

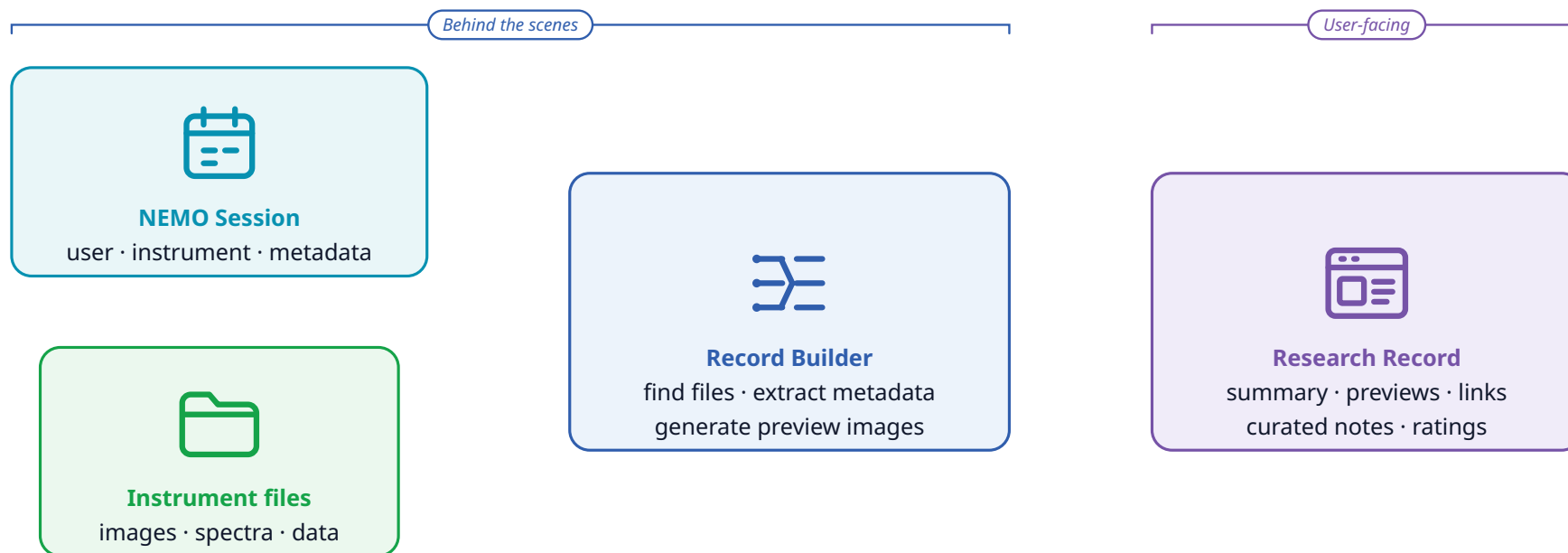
- Automatically links scheduling records (NEMO) to raw data files
- Extracts metadata from instrument-specific file formats
- Stores structured, searchable experiment records in a web-accessible database

Why it matters:

- No manual metadata entry required
- Full provenance: who, what instrument, when, and what data
- Supports FAIR data principles for long-term reuse

What does NexusLIMS do?

Combines facility context + scientific data to create reusable research records:



How a NEMO session becomes a record

NEMO provides the crucial **physical-to-digital bridge** needed to pair real-world sessions with digital data.

NEMO SESSION DATA

Instrument

tool

Actual start and end times

Usage event start / end times

Authenticated user

user (with institutional username)

Usage metadata

Pre/post-run and reservation
question answers

HOW NEXUSLIMS USES IT

Select data directory

Use that instrument's configured data directory.

Matching files

Find parseable files modified during the actual session window.

Ownership and access

Assign a user and apply configured access controls.

Experiment context

Add user, sample, purpose, elemental information, and
supplied metadata to the summary.

Each usage event becomes one searchable record

1 Summary/abstract display

The landing view shows session info, core metadata, and a preview image gallery.

2 Per-dataset file viewer

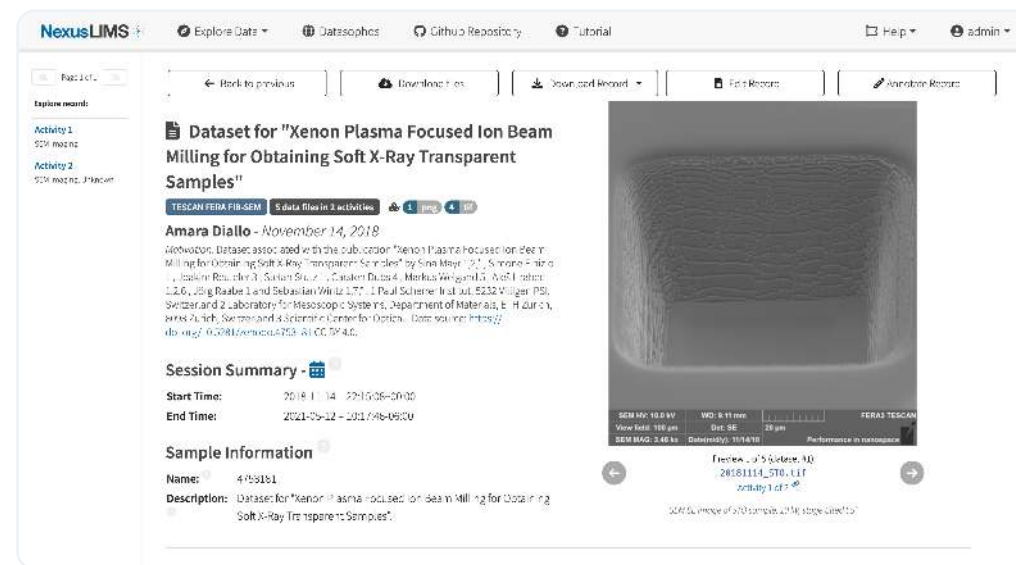
View individual dataset tables with previews and detailed metadata further down the page.

3 View (proprietary) scientific metadata

All extracted metadata for every file is contained in the record for searching (or LLM use).

4 Download underlying data files

Quickly download all dataset files associated with the record (within reason).



Example experiment record in the NexusLIMS web interface

Each usage event becomes one searchable record

1

Summary/abstract display

The landing view shows session info, core metadata, and a preview image gallery.

2

Per-dataset file viewer

View individual dataset tables with previews and detailed metadata further down the page.

3

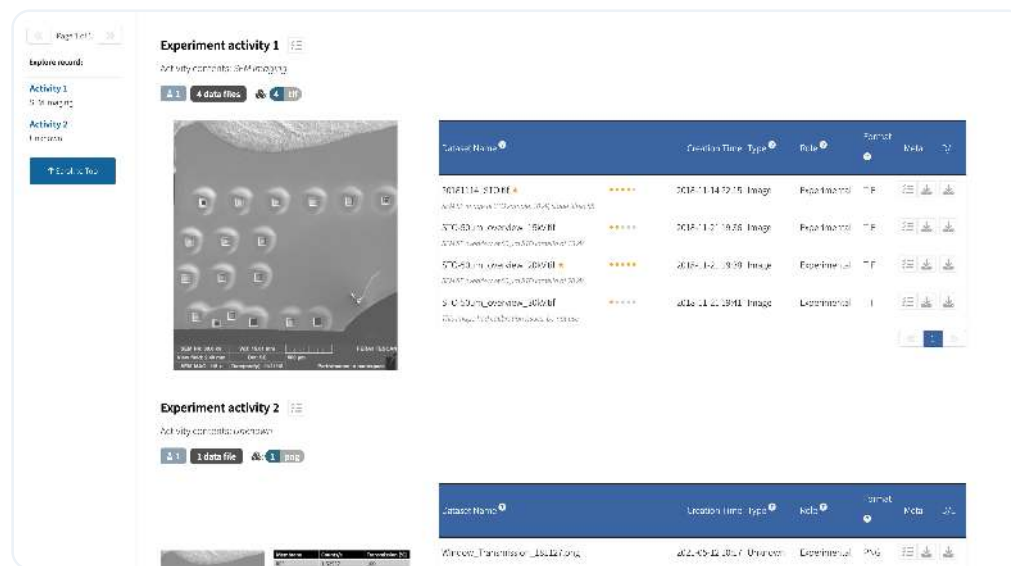
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Example experiment record in the NexusLIMS web interface

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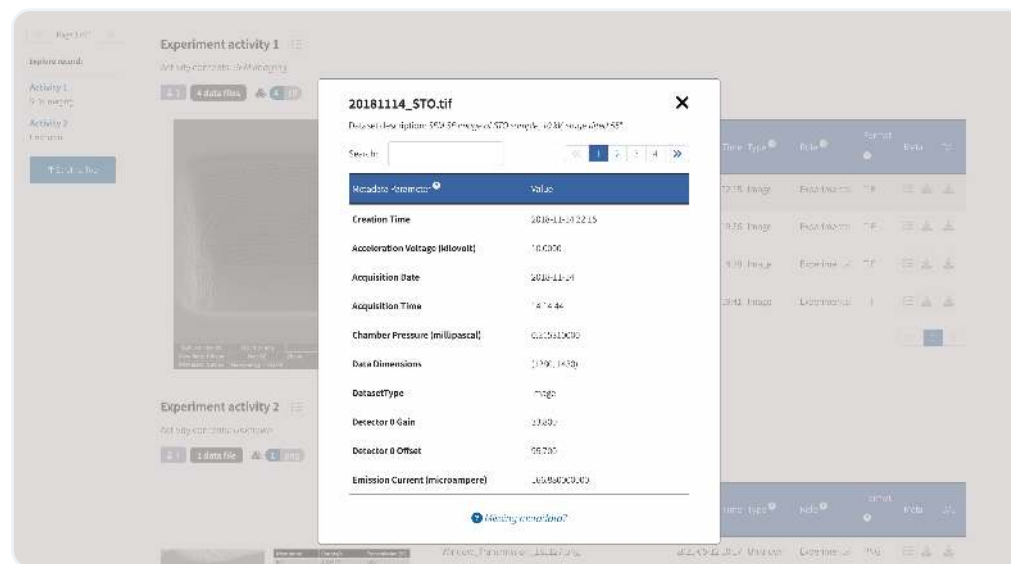
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Example experiment record in the NexusLIMS web interface

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The landing view shows session info, core metadata, and a preview image gallery.

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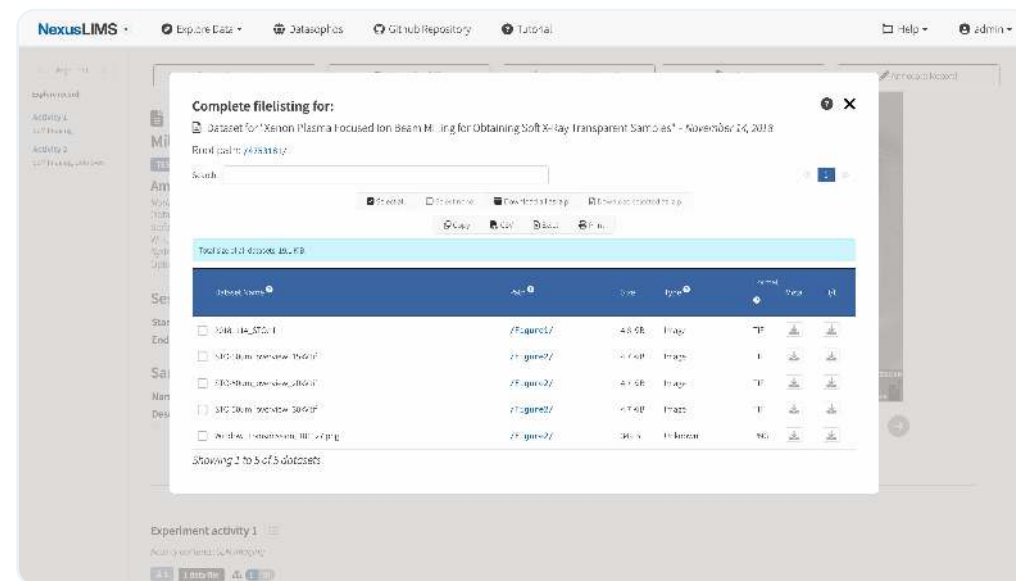
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All extracted metadata for every file is contained in the record for searching (or LLM use).

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Quickly download all dataset files associated with the record (within reason).



Example experiment record in the NexusLIMS web interface

Easily search all experiments from your facility

The screenshot displays the NexusLIMS web interface. At the top, there is a navigation bar with links for 'Explore Data', 'Datasophos', 'Github Repository', and 'Tutorial'. A search bar is prominently featured with the placeholder text 'Enter keywords, or leave blank to retrieve all records' and a 'Search' button. Below the search bar, it indicates 'Found 21 results:'. Three results are listed, each with a checkbox, a title, a brief description, and a date. The first result is 'The microstructure and He+ ion irradiation behavior of novel low-activation W-Ta-Cr-V refractory high entropy alloy for nuclear applications' by Luca Ferretti, dated June 02, 2022. The second is 'EELS and EDS maps of YAlO3' by Marcus Webb, dated March 27, 2026. The third is 'Virus – calcium carbonate composites: Possible mechanisms of bacteriophage-induced vaterite formation - Dataset' by Yuki Tanaka, dated January 31, 2024. Each result includes file format tags (e.g., bmp, dm3, dm4, tif) and a 'Data' button.

1

Browse all records

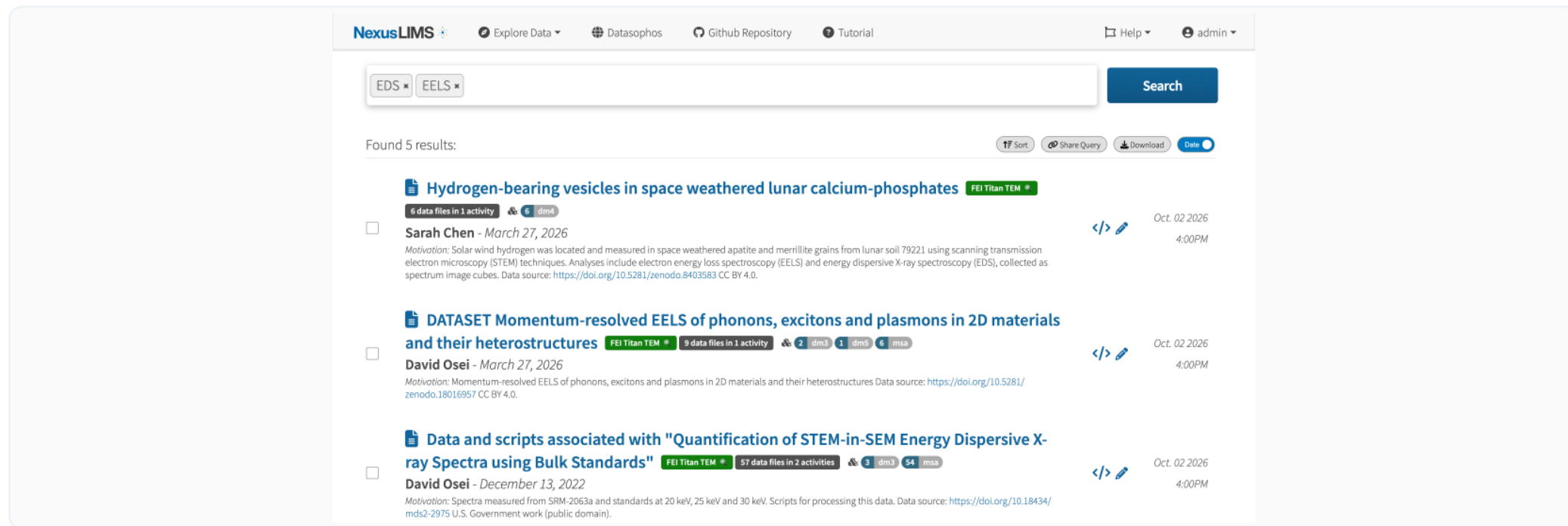
2

Search by arbitrary keyword

3

Refine with filters

Easily search all experiments from your facility



The screenshot displays the NexusLIMS web application interface. At the top, there is a navigation bar with the NexusLIMS logo, links for 'Explore Data', 'Datasophos', 'Github Repository', and 'Tutorial', along with a 'Help' dropdown and a user profile 'admin'. Below the navigation bar is a search section with a text input field containing 'EDS' and 'EELS', a 'Search' button, and a 'Found 5 results:' indicator. To the right of the search bar are buttons for 'Sort', 'Share Query', 'Download', and 'Data'. The search results are listed below, each with a checkbox, a title, a date, a motivation, and a data source. The first result is 'Hydrogen-bearing vesicles in space weathered lunar calcium-phosphates' by Sarah Chen, dated March 27, 2026. The second result is 'DATASET Momentum-resolved EELS of phonons, excitons and plasmons in 2D materials and their heterostructures' by David Osei, dated March 27, 2026. The third result is 'Data and scripts associated with "Quantification of STEM-in-SEM Energy Dispersive X-ray Spectra using Bulk Standards"' by David Osei, dated December 13, 2022. Each result also includes a 'FEI Titan TEM' badge and a '6 data files in 1 activity' badge.

NexusLIMS Explore Data Datasophos Github Repository Tutorial Help admin

EDS EELS Search

Found 5 results: Sort Share Query Download Data

☐ **Hydrogen-bearing vesicles in space weathered lunar calcium-phosphates** FEI Titan TEM 6 data files in 1 activity 6 dm4 Sarah Chen - March 27, 2026 Oct. 02 2026 4:00PM
Motivation: Solar wind hydrogen was located and measured in space weathered apatite and merrillite grains from lunar soil 79221 using scanning transmission electron microscopy (STEM) techniques. Analyses include electron energy loss spectroscopy (EELS) and energy dispersive X-ray spectroscopy (EDS), collected as spectrum image cubes. Data source: <https://doi.org/10.5281/zenodo.8403583> CC BY 4.0.

☐ **DATASET Momentum-resolved EELS of phonons, excitons and plasmons in 2D materials and their heterostructures** FEI Titan TEM 9 data files in 1 activity 2 dm3 1 dm5 6 msa David Osei - March 27, 2026 Oct. 02 2026 4:00PM
Motivation: Momentum-resolved EELS of phonons, excitons and plasmons in 2D materials and their heterostructures Data source: <https://doi.org/10.5281/zenodo.18016957> CC BY 4.0.

☐ **Data and scripts associated with "Quantification of STEM-in-SEM Energy Dispersive X-ray Spectra using Bulk Standards"** FEI Titan TEM 57 data files in 2 activities 3 dm3 54 msa David Osei - December 13, 2022 Oct. 02 2026 4:00PM
Motivation: Spectra measured from SRM-2063a and standards at 20 keV, 25 keV and 30 keV. Scripts for processing this data. Data source: <https://doi.org/10.18434/mds2-2975> U.S. Government work (public domain).

1 Browse all records

2 Search by arbitrary keyword

3 Refine with filters

Easily search all experiments from your facility

The screenshot displays the NexusLIMS web interface. At the top, there is a navigation bar with links for 'Explore Data', 'Datasophos', 'Github Repository', and 'Tutorial'. A search bar contains the text 'instrument-pid:FEI-Quanta-SEM' and a 'Search' button. Below the search bar, it indicates 'Found 2 results:'. Two results are listed:

- SEM images of PAAO samples (AJ series 1-to-5)** by Amara Diallo - March 27, 2026. The description mentions scanning electron microscopy (SEM) images of porous anodized aluminum oxide (PAAO) samples. It includes a '15 data files in 1 activity' tag and a '15 tif' file count. The date is 'Oct. 02 2026 4:00PM'.
- Demo datasets used by the openECCI Python library** by Thomas Kirchner - December 19, 2022. The description mentions demo datasets used by the openECCI Python library for Electron Channelling Contrast Imaging (ECCI) analysis. It includes a '51 data files in 2 activities' tag and a '51 tif' file count. The date is 'Oct. 02 2026 4:00PM'.

1 Browse all records

2 Search by arbitrary keyword

3 Refine with filters

NexusLIMS project history

Most features shown so far, such as NEMO integration, record building, metadata extraction, previews, and the CDCS frontend, were implemented (*by me*) during the NIST era.

NIST foundations

2020–2023

Developed the core workflows: NEMO session harvesting, file matching, metadata extraction, previews, and searchable records.

Published in [Microscopy & Microanalysis](#) in 2021.

Feature pause

After 2023

Feature development effectively ended in 2023. The most recent NIST release ([v1.4.3](#)) followed in June 2024; the NIST deployment is still running.

NexusLIMS 2.0!

Since December 2025

With UPenn/Singh Center support, Datasophos formally forked NexusLIMS in December 2025 to add many new features and better support deployment at other institutions.

What has changed in NexusLIMS 2.0+?

Many improvements for both administrators and researchers:

Easier deployment

- One-command install and guided setup
- Documented web deployment

More instrument support

- More file formats and rich previews
- Extensible instrument plugins

More export options

- CDCS, eLabFTW, and LabArchives
- Custom export plugins

Richer user features

- Edit records; curate and feature datasets
- Per-user ownership and access settings

Easy install and deployment (Record builder *backend*)

1 Install the record builder with one command

```
uv tool install nexuslims
```

2 Interactive configuration wizard

```
nexuslims config edit
```

One place to configure all NexusLIMS settings.

3 Instrument management tool

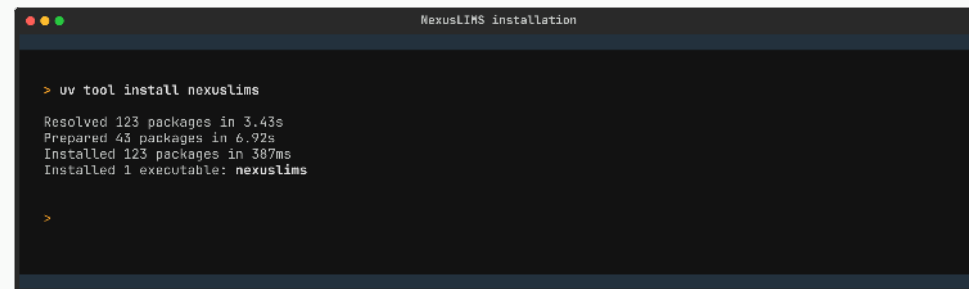
```
nexuslims instruments manage
```

Add, edit, or remove instruments from NexusLIMS.

4 Build

```
nexuslims build-records
```

Simple command to build records (typically on a schedule).



```
NexusLIMS installation

> uv tool install nexuslims

Resolved 123 packages in 3.43s
Prepared 43 packages in 6.92s
Installed 123 packages in 387ms
Installed 1 executable: nexuslims

>
```

Installing the record builder with uv

Easy install and deployment (Record builder *backend*)

1 Install the record builder with one command

`uv tool install nexuslims`

2 Interactive configuration wizard `nexuslims config edit`

One place to configure all NexusLIMS settings.

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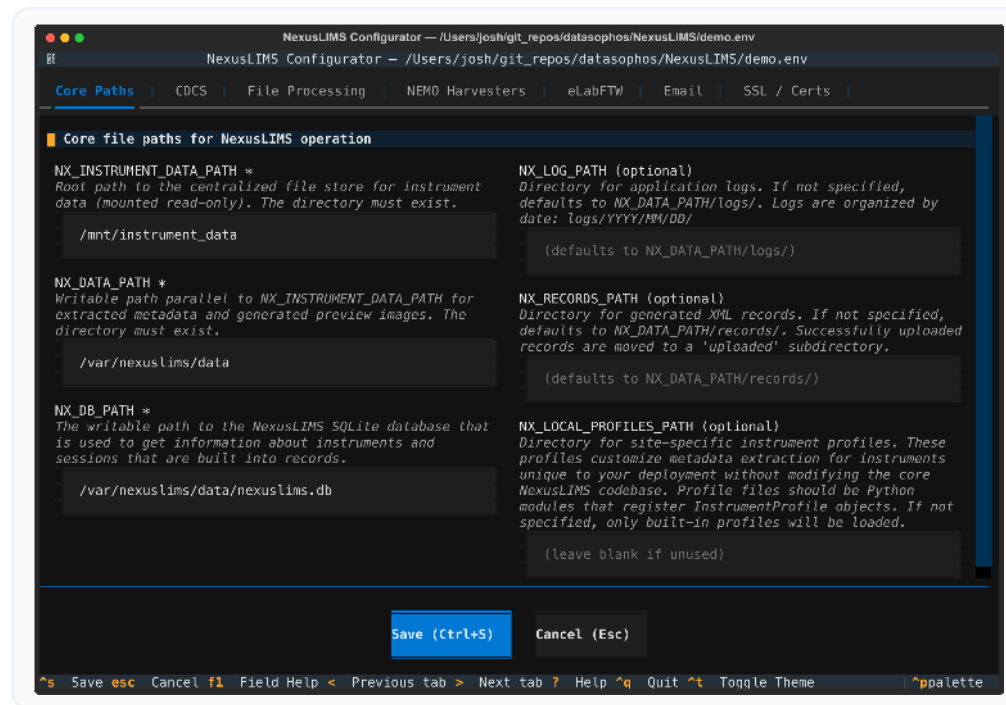
`nexuslims instruments manage`

Add, edit, or remove instruments from NexusLIMS.

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Simple command to build records (typically on a schedule).



Configure NexusLIMS with guided inline help

Easy install and deployment (Record builder *backend*)

1 Install the record builder with one command

`uv tool install nexuslims`

2 Interactive configuration wizard

`nexuslims config edit`

One place to configure all NexusLIMS settings.

3 Instrument management tool

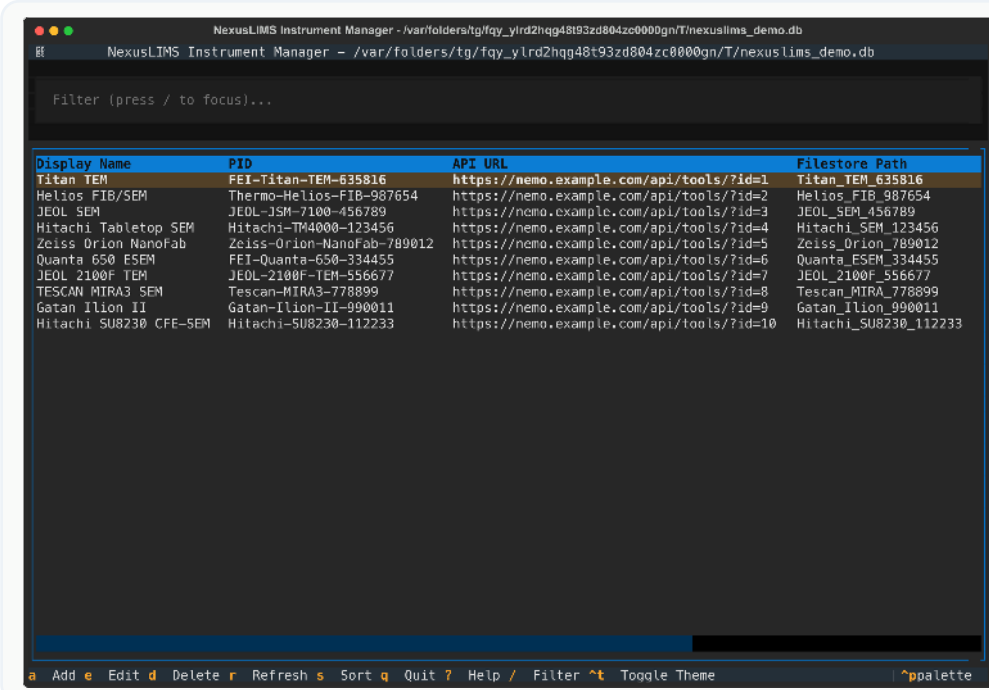
`nexuslims instruments manage`

Add, edit, or remove instruments from NexusLIMS.

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`nexuslims build-records`

Simple command to build records (typically on a schedule).



The screenshot shows a terminal window titled "NexusLIMS Instrument Manager - /var/folders/tg/fqy_yld2hgg48t93zd804zc0000gn/T/nexuslims_demo.db". The interface displays a table of instruments with columns: Display Name, PID, API URL, and Filestore Path. The table lists various instruments like Titan TEM, Helios FIB/SEM, JEOL SEM, Hitachi Tabletop SEM, Zeiss Orion NanoFab, Quanta 650 ESEM, JEOL 2100F TEM, TESCAN MIRA3 SEM, Gatan Ilion II, and Hitachi SU8230 CFE-SEM. At the bottom, there is a status bar with icons and text: "a Add e Edit d Delete r Refresh s Sort q Quit ? Help / Filter ^t Toggle Theme ^ppalette".

Display Name	PID	API URL	Filestore Path
Titan TEM	FEI-Titan-TEM-835816	https://nemo.example.com/api/tools/?id=1	Titan_TEM_635816
Helios FIB/SEM	Thermo-Helios-FIB-987654	https://nemo.example.com/api/tools/?id=2	Helios_FIB_987654
JEOL SEM	JEOL-JSM-7100-456789	https://nemo.example.com/api/tools/?id=3	JEOL_SEM_456789
Hitachi Tabletop SEM	Hitachi-TM4000-123456	https://nemo.example.com/api/tools/?id=4	Hitachi_SEM_123456
Zeiss Orion NanoFab	Zeiss-Orion-NanoFab-789012	https://nemo.example.com/api/tools/?id=5	Zeiss_Orion_789012
Quanta 650 ESEM	FEI-Quanta-650-334455	https://nemo.example.com/api/tools/?id=6	Quanta_ESEM_334455
JEOL 2100F TEM	JEOL-2100F-TEM-556677	https://nemo.example.com/api/tools/?id=7	JEOL_2100F_556677
TESCAN MIRA3 SEM	Tescan-MIRA3-778899	https://nemo.example.com/api/tools/?id=8	Tescan_MIRA_778899
Gatan Ilion II	Gatan-Ilion-II-990011	https://nemo.example.com/api/tools/?id=9	Gatan_Ilion_990011
Hitachi SU8230 CFE-SEM	Hitachi-SU8230-112233	https://nemo.example.com/api/tools/?id=10	Hitachi_SU8230_112233

Manage instruments in the terminal interface

Easy install and deployment (Record builder *backend*)

1 Install the record builder with one command

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uv tool install nexuslims
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```

One place to configure all NexusLIMS settings.

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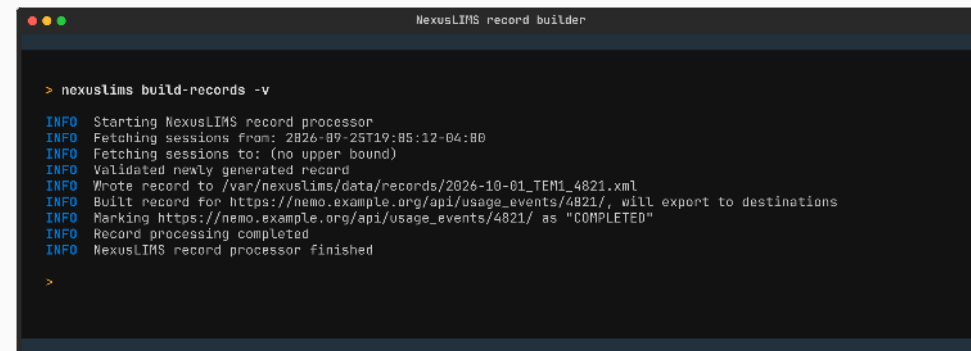
```
nexuslims instruments manage
```

Add, edit, or remove instruments from NexusLIMS.

4 Build

```
nexuslims build-records
```

Simple command to build records (typically on a schedule).

A terminal window titled "NexusLIMS record builder" showing the output of the command "nexuslims build-records -v". The output is as follows:

```
> nexuslims build-records -v
INFO Starting NexusLIMS record processor
INFO Fetching sessions from: 2826-89-25T19:05:12-04:00
INFO Fetching sessions to: (no upper bound)
INFO Validated newly generated record
INFO Wrote record to /var/nexuslims/data/records/2026-10-01_TEM1_4821.xml
INFO Built record for https://nemo.example.org/api/usage_events/4821/, will export to destinations
INFO Marking https://nemo.example.org/api/usage_events/4821/ as "COMPLETED"
INFO Record processing completed
INFO NexusLIMS record processor finished
>
```

Build records on demand or on a schedule

Easy install and deployment (Web *frontend*)

A documented deployment stack with admin tools.

Deploy and initialize

- Docker Compose deployment
- **admin-init** automates initial setup

Configure for your facility

- One `.env` file for site settings
- Easily customize branding, logo, and style

Built-in web server

- HTTPS served by Caddy
- Automatic or institutional certificates

Maintain and upgrade

- Backup, restore, and diagnostics
- Automated schema and record upgrades

[Production deployment guide](#) [↗] · [Administration reference](#) [↗]

Supported microscopy file formats

Scientific metadata extraction and preview generation

Format	Extension(s)	Data types	Added
Gatan DigitalMicrograph	.dm3, .dm4	TEM/STEM imaging, diffraction, EELS/EDS spectra	1.0
FEI/Thermo Fisher SEM/FIB	.tif	SEM and FIB imaging	2.0
Zeiss Orion / Fibics HIM	.tif	Helium ion imaging	2.0
Tescan (P)FIB/SEM	.tif	SEM and FIB imaging	2.0
FEI TIA	.ser, .emi	TEM/STEM imaging, diffraction, EELS/EDS spectra	1.0
EDAX / EMSA-MAS	.spc, .msa	EDS spectra	1.0
Tofwerk fibTOF pFIB-ToF-SIMS	.h5	pFIB-ToF-SIMS spectrum images	2.0

Preview only: Images (.png, .jpg, .tiff, .bmp, .gif) get basic metadata and thumbnail previews; .txt files also get a text-to-image preview.

Other files: Unknown formats retain their timestamp and get a placeholder preview.

New user features

Annotation · Curation · Featured gallery · User ownership

[Feature documentation](#) 

Annotating records

The screenshot displays the NexusLIMS web interface. The main panel shows a dataset record titled "Dataset for 'Xenon Plasma Focused Ion Beam Milling for Obtaining Soft X-Ray Transparent Samples'". It includes a session summary with start and end times, and sample information. On the right, an "Annotate Record" sidebar is open, showing a list of files with their thumbnails and descriptions. The files are: 20181114_STO.tif, STO-50um_overview_15kv.tif, STO-50um_overview_20kv.tif, and STO-50um_overview_30kv.tif. The sidebar also shows a "Window Transmission 181127.png" file. At the bottom of the sidebar, there are "Save Annotations" and "Cancel" buttons.

NexusLIMS Explore Data Datasophos Github Repository Tutorial Help admin

Explore record: Page 1 of 1

Activity 1 SEM Imaging
Activity 2 Unknown

Dataset for "Xenon Plasma Focused Ion Beam Milling for Obtaining Soft X-Ray Transparent Samples"

TESCAN FERA FIB-SEM 5 data files in 2 activities 1 png 4 tif

Amara Diallo - November 14, 2018

Motivation: Dataset associated with the publication "Xenon Plasma Focused Ion Beam Milling for Obtaining Soft X-Ray Transparent Samples" by Sina Mayr 1,2*, Simone Fritzsche 1, Joakim Reuter 3, Stefan Stutz 1, Carsten Dubs 4, Markus Weigand 5, Aleš Hrabec 1,2,6, Jörg Raabe 1 and Sebastian Wintz 1,7*, 1 Paul Scherrer Institut, 5232 Villigen PSI, Switzerland 2 Laboratory for Mesoscopic Systems, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland 3 Scientific Center for Optics... Data source: <https://doi.org/10.5281/zenodo.4753181> CC BY 4.0.

Session Summary

Start Time: 2018-11-14 - 22:15:08+00:00
End Time: 2021-09-12 - 10:17:46-06:00

Sample Information

Name: 4753181
Description: Dataset for "Xenon Plasma Focused Ion Beam Milling for Obtaining Soft X-Ray Transparent Samples"

Annotate Record

Use this panel to add or edit descriptions for each dataset. You can also click **Edit Record** in the top bar to open the full editor where you can add/edit samples, create/delete activities, reassign datasets, and more.

ACTIVITY 1

- 20181114_STO.tif** SEM SE image of STO sample. 10 kv, stage tilted 55°
- STO-50um_overview_15kv.tif** SEM SE overview of 50 µm STO lamella at 15 kv
- STO-50um_overview_20kv.tif** SEM SE overview of 50 µm STO lamella at 20 kv
- STO-50um_overview_30kv.tif** This image had calibration issues. Do not use

ACTIVITY 2

- Window Transmission 181127.png**

Save Annotations Cancel

Adding dataset descriptions

- Automated harvesting and extraction cannot capture rich researcher-written metadata
- The annotator feature allows you to quickly and easily add free-text descriptions to each dataset, adding context to your experimental record
- Accessible as a sidebar panel on the record display page or inline for each dataset

Record editing and curation

1 · Edit

2 · Samples

3 · Review

4 · Featured datasets

[Documentation](#)

The screenshot shows the 'Edit/Annotate Record' page in NexusLIMS. At the top, there's a navigation bar with 'NexusLIMS', 'Explore Data', 'Datasophos', 'Github Repository', and 'Tutorial'. Below this, the page title 'Edit/Annotate Record' is followed by buttons for 'Edit XML', 'Help', and 'Back to Record'. A descriptive paragraph explains the purpose of the page: to add descriptions to datasets, add images, and use the selection tool to assign datasets to different activities. The main content area shows a record titled 'Dataset for "Mercury Plasma Focused on Beam Milling" or "Obtaining Soft X-Ray Transparent Samples"'. It lists three activities: 'SEM SE image of STO sample, 10 kv, slope tilted 55°', 'SEM SE overview of 50 µm STO lamella at 15 kv', and 'SEM SE overview of 50 µm STO lamella at 20 kv'. Each activity has a corresponding image thumbnail. Below the activities, there's a section for 'Window Transmission_181127.png' with a description field. At the bottom, there are buttons for 'Save To DB', 'Cancel', and '+ Add Activity'.

Edit the record

The full-page record editor allows you to revise the title and dataset descriptions, add or edit activities, and move datasets between activities by dragging and dropping them.

Record editing and curation

1 · Edit

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[Documentation](#)

The screenshot shows a 'Add Sample' dialog box with the following fields and options:

- Name ***: A text input field with the placeholder 'A new sample'.
- Persistent Identifier (PID)**: A text input field containing 'https://doi.org/10.1234/example'.
- Description**: A text input field with the placeholder 'This sample wasn't included in the original activity information, so I added it after!'.
- Elements**: A section with a row of element tags: Fe x, Cr x, Cu x, Ni x. Below this is a text input field with the placeholder 'Type symbol (e.g. Fe) and press Enter or comma.' and a note 'Press Enter or comma to add. Click a tag to remove it.'
- Buttons**: 'Cancel' and 'Save Sample' (highlighted with a blue border).
- Footer**: A small asterisk icon and the text '* Required'.

Manage samples

Add or update a sample's name, persistent identifier, description, and elemental composition. Assign samples to acquisition activities from each activity header.

Record editing and curation

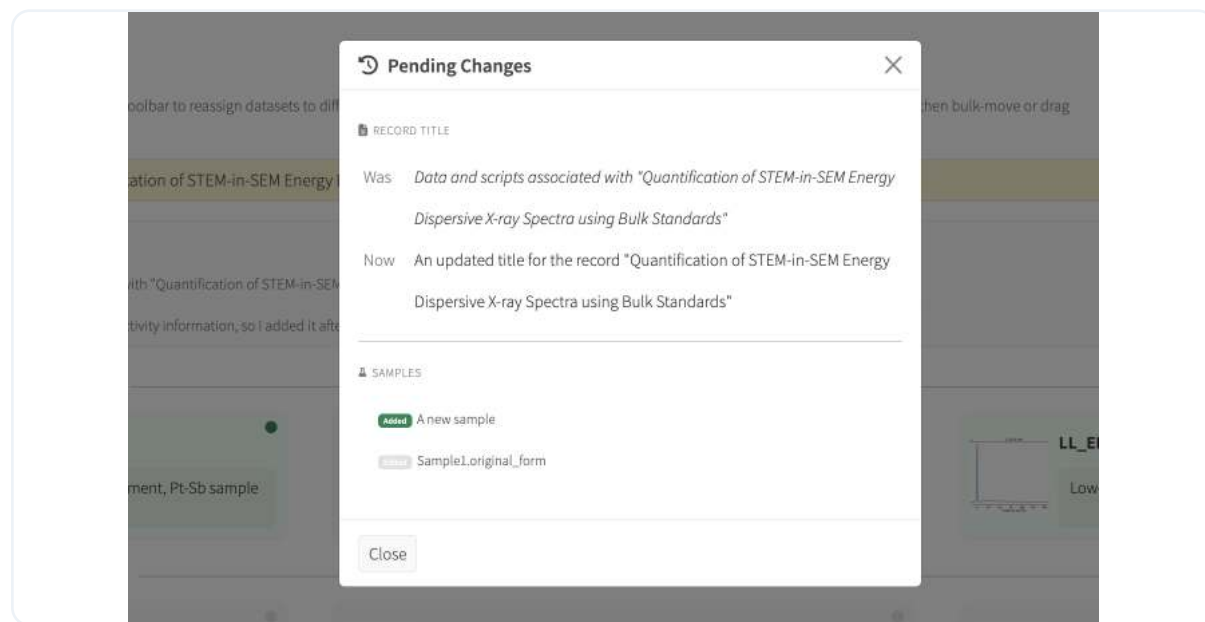
1 · Edit

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[Documentation](#)



Review changes before saving

The Pending Changes summary gathers unsaved title, description, sample, dataset-move, and activity edits before you save or navigate away.

Record editing and curation

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[Documentation](#)

Dataset Name [?]	Creation Time	Type [?]	Role [?]	Meta	D/L
curation_test_001.dm3   --- Featured and rated 3 — tests read-only display and...		Image	Experi...	 	
curation_test_002.dm3  --- Rated 5 only — tests max-fill circle display		Image	Experi...	 	
curation_test_003.dm3   --- Featured only — tests featured-without-rating di...		Image	Experi...	 	

<< 1 >>

Choose the dataset(s) to feature

Mark a dataset as featured or give it a 1–5 rating. These rankings control which previews are displayed in the public gallery, if enabled.

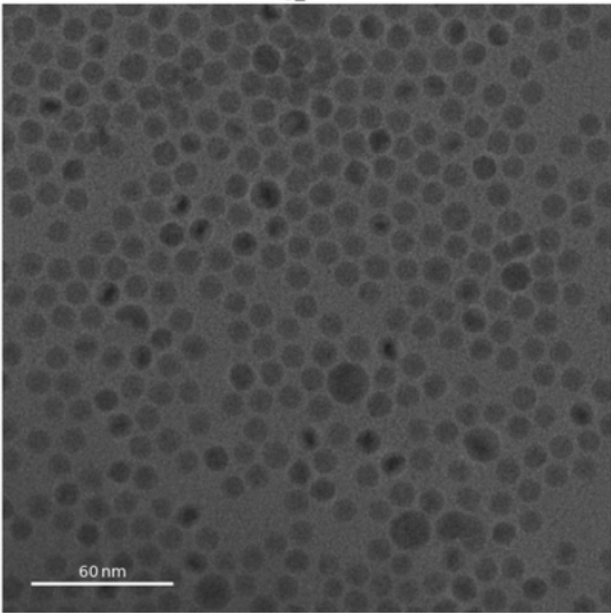
See Jamie Ford's talk tomorrow morning

Public gallery view

[Open demo gallery](#)

NexusLIMS

img_0002



60 nm

NexusLIMS

Catalytic reactivity of Glucose-coated FeO@Fe₃O₄ Nanoparticles for biomedical applications: safety assessment using a 3D hepatic in vitro model

Dataset: TEM image of FeO@Fe₃O₄ nanoparticles at 40,000x

★ FEATURED | T. Kirchner · FEI Titan TEM · August 2023

[View record](#)

Two options for record ownership and data permissions

One open science collection

DEFAULT



All data visible to all users

The only option before recent changes.



Each record has one owner

ADDED IN v2.7.0



Each record is assigned to the researcher identified by the **NEMO usage event**.

Facilities choose record visibility:



Public workspace



Owner's private space

HOW NEMO POWERS NEXUSLIMS OWNERSHIP:

NEMO usage event

Session identifies the researcher



NexusLIMS

Matches or creates the CDCS account



CDCS record

Assigns that account as owner

If account lookup fails, the record still uploads under the administrative account and a warning is logged.

What do I need to get started with NexusLIMS?

1 • Data share

Instrument data on a central network share. One folder per instrument.

```
share/  
  microscope-A/...  
  microscope-B/...
```

Any structure inside each folder.

2 • NEMO

A running deployment with API access and a token.

Usage events supply session times, instrument identity, and the user.

3 • Server or VM



Linux (preferred) or macOS

Read access to the data share.

Writable storage for previews, extracted metadata, and the tracking database.

Install the record builder with
`uv tool install nexuslims.`

4 • Record destination



NexusLIMS-CDCS web app (default)

Docker Compose; can run on the same server.

Upload API credentials and read access to instrument data and generated metadata.

First-time setup: Map NEMO tools to folders, initialize the database, configure record builder options, and schedule record building.

[Getting started](#) · [Configuration](#) · [Web deployment \(DNS, HTTPS, backups\)](#)

A quick demo (if time allows)

1 · Show the setup path

Open the configuration wizard's NEMO settings and the instrument manager.

2 · Show the web frontend

Open a record, point out the NEMO session context, file previews, and extracted metadata.

3 · Show user curation

Show an annotation example, then open the public visual gallery.

Live demo

nexuslims-demo.datasophos.co

Thank you!

A brief plug...

If you need assistance deploying or configuring NexusLIMS
(or any other data services), please reach out!

[Documentation](#) · [GitHub](#) · josh@datasophos.co

Reference: Record building workflow

A scheduled run turns completed instrument sessions into searchable experiment records.

- 1 Discover pending sessions**
Poll NEMO usage events; identify sessions awaiting a record.
- 2 Gather experiment context**
Harvest user, sample, and purpose metadata; check data consent.
- 3 Match the data files**
Search the instrument's configured folder for files modified within the session window.
- 4 Group acquisition activities**
Use gaps between file timestamps to infer activity boundaries.
- 5 Extract and organize metadata**
Generate JSON metadata and PNG previews. Separate shared setup parameters from values that vary by dataset.
- 6 Validate and upload**
Build schema-validated XML, upload to CDCS, and update the session's processing status.

NEMO metadata priority: Post-run answers → pre-run answers → matching reservation. Each source is checked for valid data and consent.

Skipped or failed sessions: No consent or no matching files → no record. Build or validation errors are logged for investigation.

[Full record building guide](#) 

Reference: NEMO question setup

Where to configure questions

In **Detailed Administration**, configure **Tool usage questions** for pre-run or post-run answers, or **Reservation questions** for booking answers. Apply the questions to the relevant tools.

NexusLIMS prefers post-run answers, then pre-run answers, then a matching reservation. A usable source must include affirmative consent.

Use these question names

data_consent
experiment_title
experiment_purpose
project_id
sample_group

Required consent
Record title
Experiment context
Project identifier
Repeatable sample information

[NEMO question configuration and examples](#) 

Minimal consent question

```
[
  {
    "type": "radio",
    "name": "data_consent",
    "title": "Allow data curation?",
    "choices": ["Agree", "Disagree"],
    "required": true
  }
]
```

Inside each sample group:

sample_name, sample_or_pid,
sample_details, sample_elements.

Display labels can be customized; keep the expected name values.

Reference: File selection and timing

Files must be in the instrument's configured folder, with modification times inside the actual usage window.

Which files are included?

`NX_FILE_STRATEGY`

- `exclusive` (default): Include formats with a dedicated metadata extractor.
- `inclusive`: Also include other formats, with basic filesystem metadata.

`NX_IGNORE_PATTERNS` excludes matching names under either strategy. Use it for temporary files, sidecars, or unwanted large files.

What if files arrive later?

`NX_FILE_DELAY_DAYS` (default: 2)

When no files are found, subsequent scheduled runs retry until the configured window expires.

Example: A session ends Monday at 5 pm. With a two-day window, retries continue until Wednesday at 5 pm.

Later transfers still need modification times that match the session.

Missing files? Check the tool-to-folder mapping, session times/timezone, transfer timestamps, read permissions, file strategy, and ignore patterns.

[File handling configuration](#) 

Reference: Export destinations

One built record can be published to multiple configured destinations.

CDCS	eLabFTW	LabArchives
Default destination: a searchable, schema-validated experiment record with previews and links to data.	One experiment per session: a summary, tags, structured metadata, and the XML record attached.	One notebook page per session: an HTML summary and attached XML, organized by instrument and date.

ELN summaries can link back to the CDCS record when available. Configure each destination’s URL and credentials to enable it.

Choose success criteria with NX_EXPORT_STRATEGY

all (default)	Every enabled destination must succeed.
first_success	Stop after the first successful destination.
best_effort	Attempt all; at least one success is enough.

Per-destination results are logged; exports that do not meet the strategy leave the session BUILT_NOT_EXPORTED.

[Export destinations and strategies](#)

Reference: Supporting another instrument

Choose the extension that fits the instrument's data and your facility's metadata needs.

Metadata extractor

For a new file format.

Detect supported files and parse scientific metadata into NexusLIMS fields.

Preserve native metadata alongside normalized values.

Preview generator

For a new visualization.

Turn an image, spectrum, or other measurement into a useful thumbnail.

Reuse existing preview support when it fits.

Instrument profile

For local customization.

Adjust extracted values, add static metadata or warnings, or select an extractor for a particular instrument.

Load facility profiles with
`NX_LOCAL_PROFILES_PATH`.

A practical onboarding path

1

Map the instrument

Connect its NEMO tool to its data folder.

2

Test sample files

Try representative data and acquisition modes.

3

Check the record

Verify metadata, units, timestamps, and previews.

[Developer guides: extractors, previews, and profiles](#) 

Reference: Controlled vocabularies

Consistent dataset categories and scientific terms help compare records across instruments.

Dataset classification

DatasetType has six allowed values and selects the appropriate metadata validation schema:

Image	Spectrum
SpectrumImage	Diffraction
Misc	Unknown

Technique labels (Data Type) follow naming conventions, e.g., SEM_Imaging or STEM_EELS. Additional labels are allowed.

Shared scientific terms

Standard metadata fields align with the **Electron Microscopy Glossary (EM Glossary)** where mappings exist.

Examples: acceleration_voltage, working_distance, beam_current.

Mapped schema fields carry glossary identifiers and definitions, e.g., acceleration_voltage → EMG_000000004.

Consistent units: Physical quantities are validated and converted to preferred units during XML output, e.g., 200,000 V → 200 kV.

Growing coverage: EM Glossary mappings are still developing. Vendor- and facility-specific fields can live in extensions; native file metadata is also retained.

[Dataset taxonomy](#) · [EM Glossary fields](#) · [Metadata schema and units](#)

Reference: Upgrading NexusLIMS

Release notes identify the required versions, configuration changes, and deployment steps.

1 Read both sets of release notes

Check backend/frontend compatibility and any new settings, rebuilds, or schema changes.

2 Back up the deployment

Save configuration and the backend tracking database; create a frontend backup.

3 Update the record builder

For an existing uv tool installation:

`uv tool upgrade nexuslims`

4 Apply the frontend instructions

Complete the release-specific steps, then check record building, previews, and the web interface.

Example: NexusLIMS-CDCS v3.21.0-nx1

Gallery and dataset curation release

Requires NexusLIMS backend **2.7.3 or newer**.

Condensed from its published upgrade instructions:

- 1 From deployment/, load `admin-commands.sh` and run `admin-backup`.
- 2 Retrieve the new frontend code.
- 3 Update deployment/.env:
`IMAGE_VERSION=3.21.0-nx1`
Review the optional gallery settings.
- 4 Rebuild and restart:
`dc-prod build cdc`
`dc-prod down`
`dc-prod up -d`
- 5 Run `admin-upgrade-schema` to add the schema version, update existing records, and refresh XSLT.

[Backend release example](#) · [Frontend upgrade instructions](#) · [Deployment upgrade guide](#)