Australian Synchrotron
Turning bright ideas into brilliant outcomes

A WEB-BASED USER INTERFACE FOR MX1 AND MX2 BEAMLINE DATA COLLECTION AT THE AUSTRALIAN SYNCHROTRON

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Supported by

Australian Government

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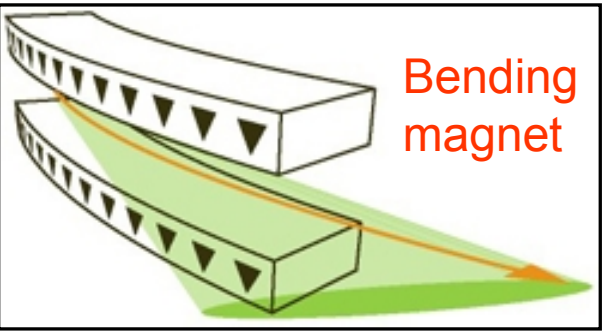
SC&IT AT THE AUSTRALIAN SYNCHROTRON

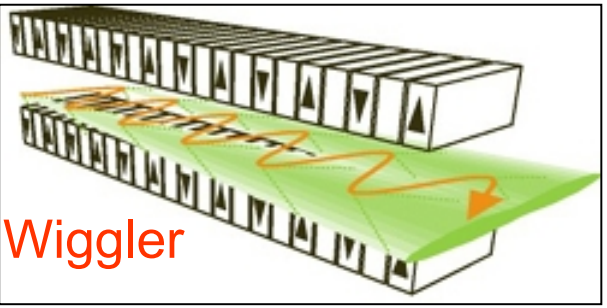
- Core IT Services
- HPC
  - MASSIVE – collaboration with Monash
- **Scientific Software Development**
  - **Automated data processing and data analysis packages**
  - **Remote access to data and instruments**

MX1/MX2 AT THE AUSTRALIAN SYNCHROTRON

Storage ring 3GeV 200mA (electrons)



Bending magnet (MX1) – high-throughput



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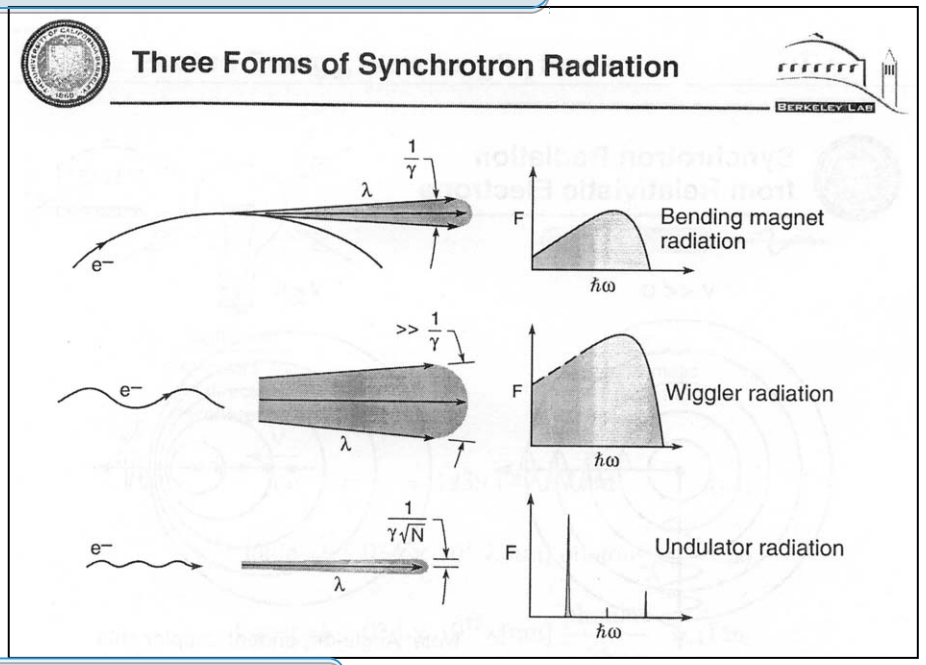

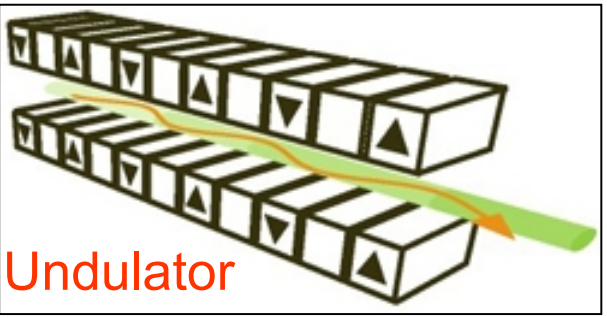

Undulator (MX2) – micro-focus

SAXS/WAXS, XFM, XAS

We have ~80% protein crystallography and ~20% chemical crystallography (more on MX1).***We focus on user support and can-do.***

MX1/MX2 AT THE AUSTRALIAN SYNCHROTRON

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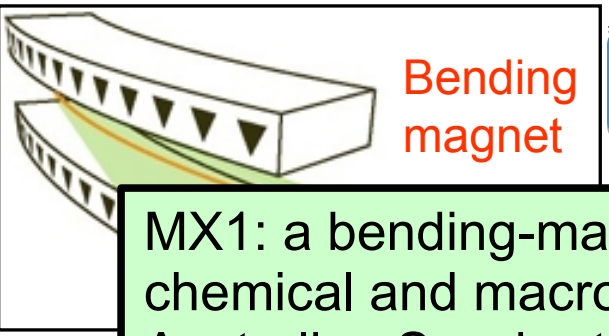
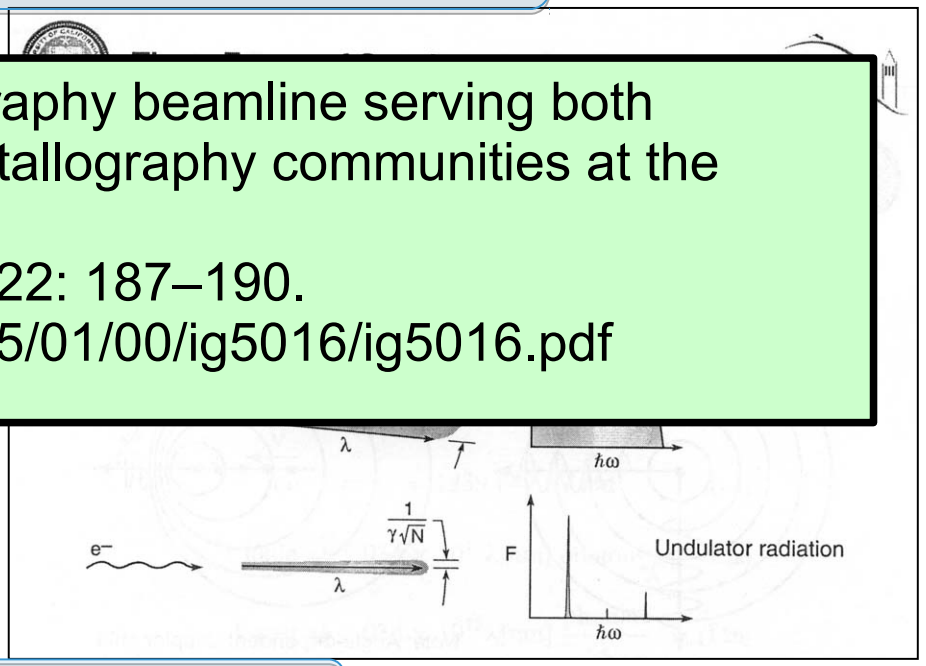
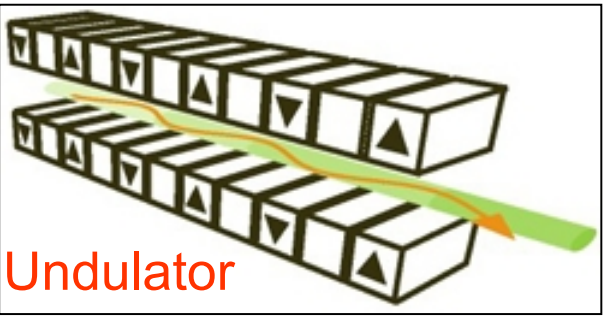


Bending magnet (MX1) – high-throughput

MX1: a bending-magnet crystallography beamline serving both chemical and macromolecular crystallography communities at the Australian Synchrotron
J Synchrotron Radiat. 2015 Jan 1; 22: 187–190.
http://journals.iucr.org/s/issues/2015/01/00/ig5016/ig5016.pdf





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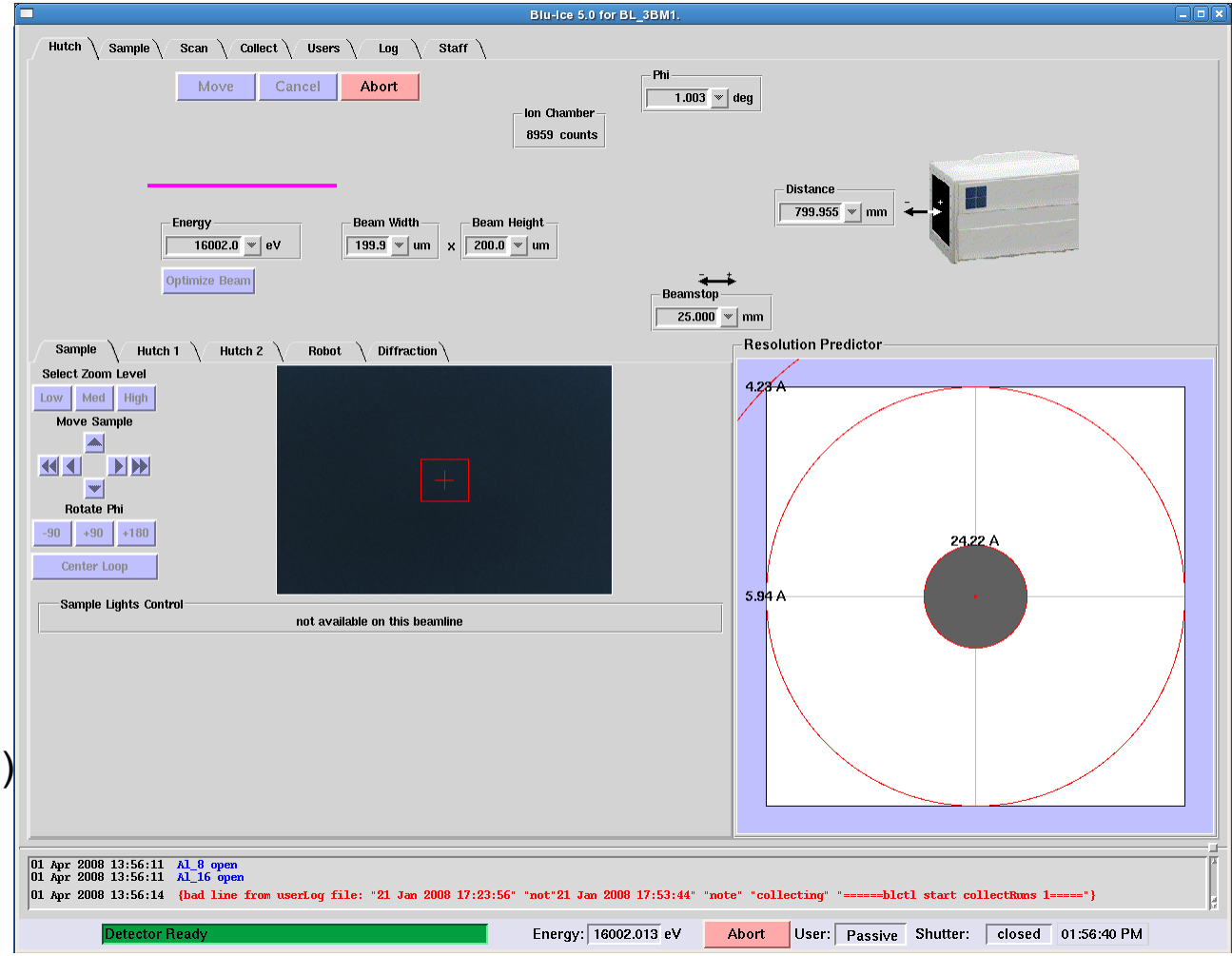
BEAMLINE DATA COLLECTION UI

- ✓Remote access via Nxclient
- ✓Excitation scans
- ✓Excitation vs F scans (MAD)
- ✓Robot sample mounting
- ✓Sample centring
- ✓Energy change control
- ✓Detector distance control
- ✓Cryo temperature control (MX1)

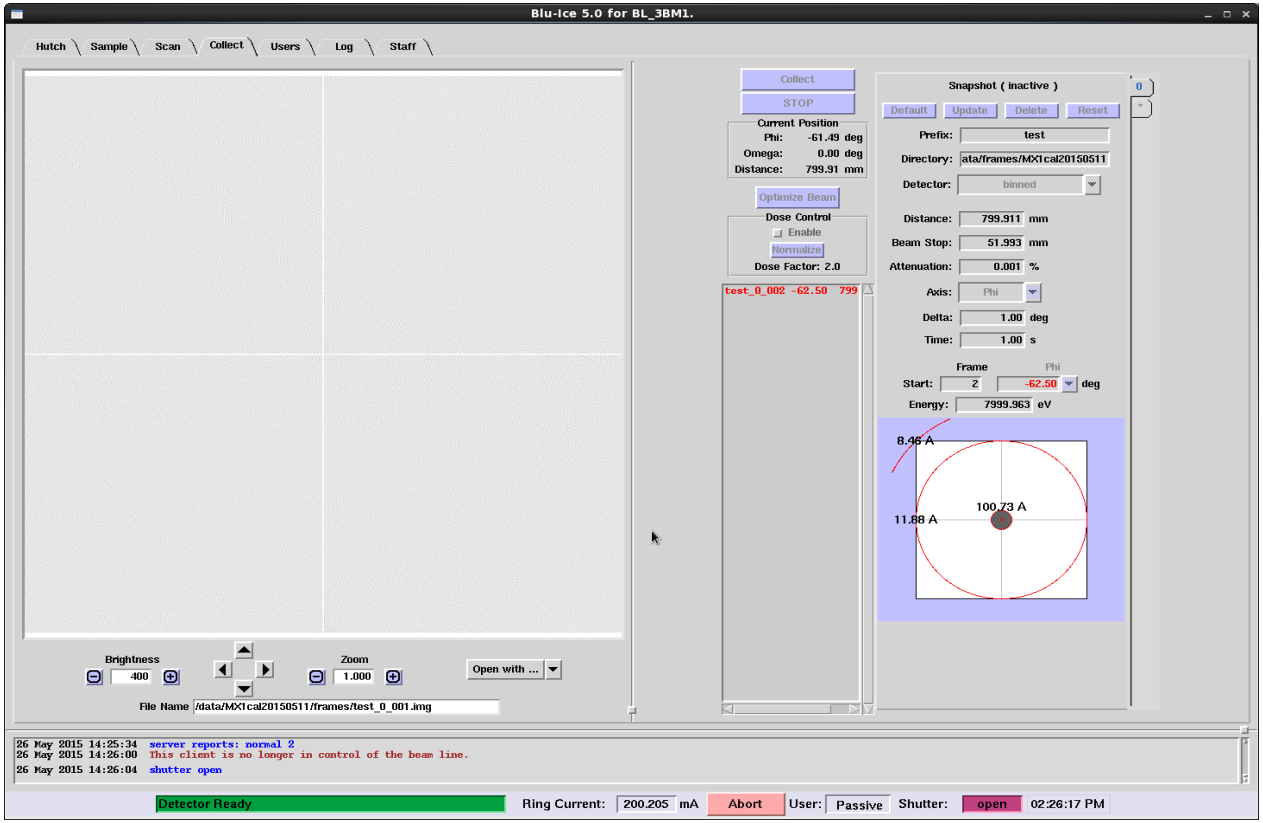


Blu-Ice

MX DATA COLLECTION - CURRENT SYSTEM

Blu-Ice

- Performance and reliability issues resulting in slower data rates and more support call-outs
- Customised, but incompatible with upstream code base.



UI PROJECT REQUIREMENTS

Yet **A**nother **I**ntegated **B**eamline **I**nterface for **X**stalography

- Utilise existing software infrastructure built at MX
  - Python Beamline library
  - Autoprocessing

- Replicate the functionality in Blu-Ice that is familiar to users:
  - Allow snapshots as well as datasets of longer runs
  - View the most recently collection diffraction image
  - Click to centre the sample

- Extendable: focus on collection tab but allow for addition of other functionality in a modular way

STANDARDISING THE TOOLKIT

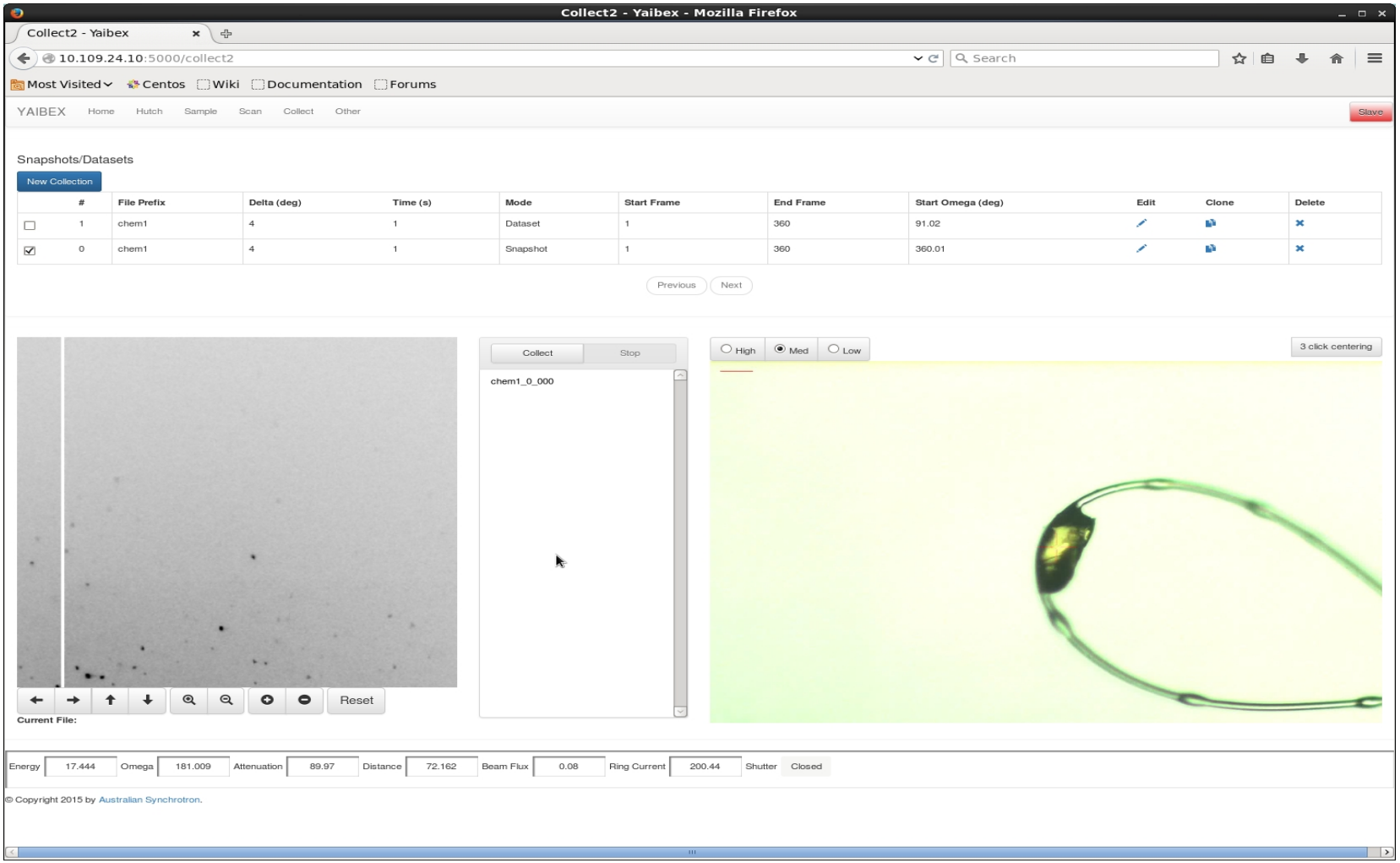
- Python as language of choice:
  - Modern language
  - Good libraries

- Flask
  - Lightweight Python web framework

- Redis
  - Key-value store

- Javascript libraries:
  - Knockout.js: MVVM javascript framework
  - Bootstrap

YAIBEX IN ACTION



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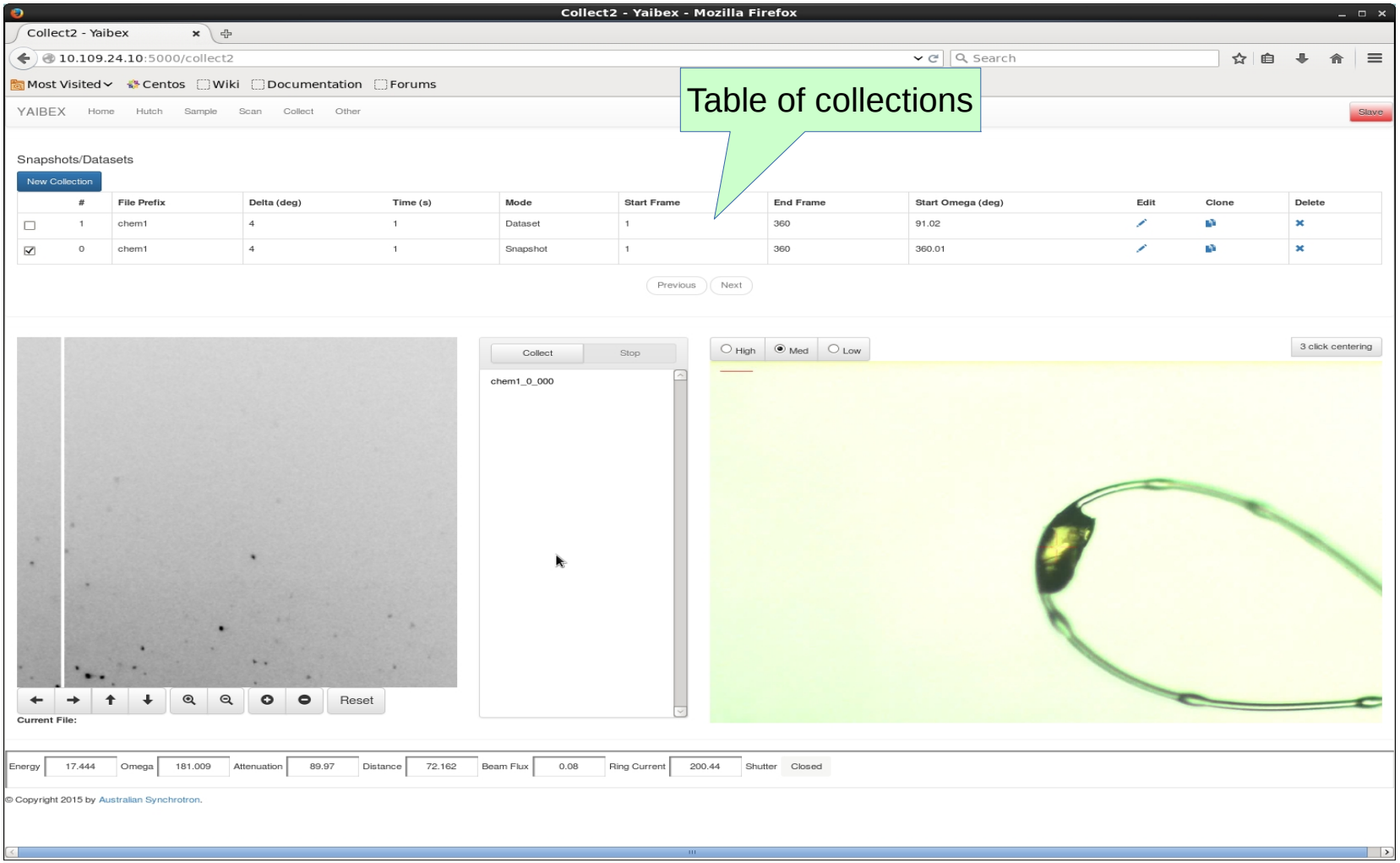

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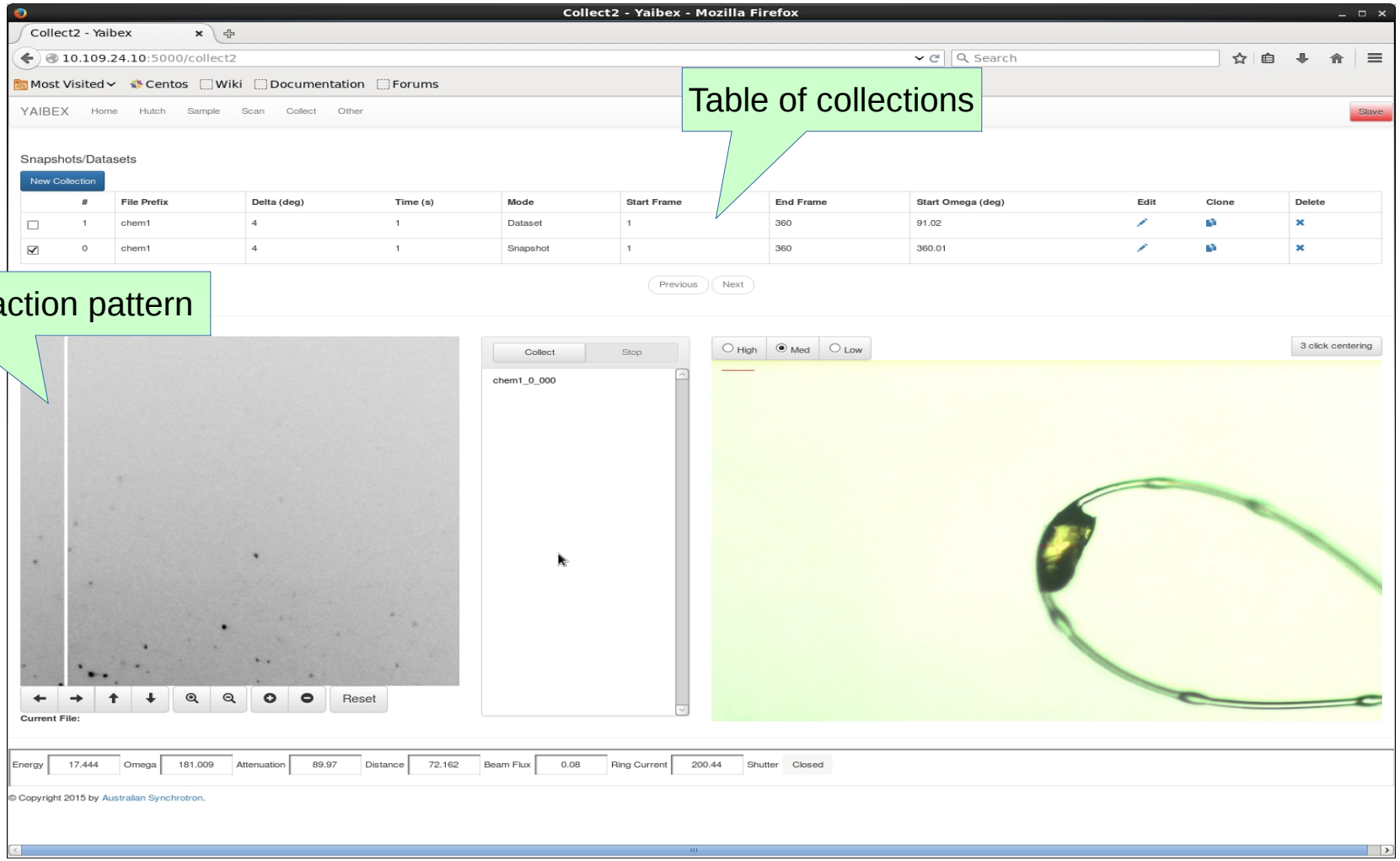

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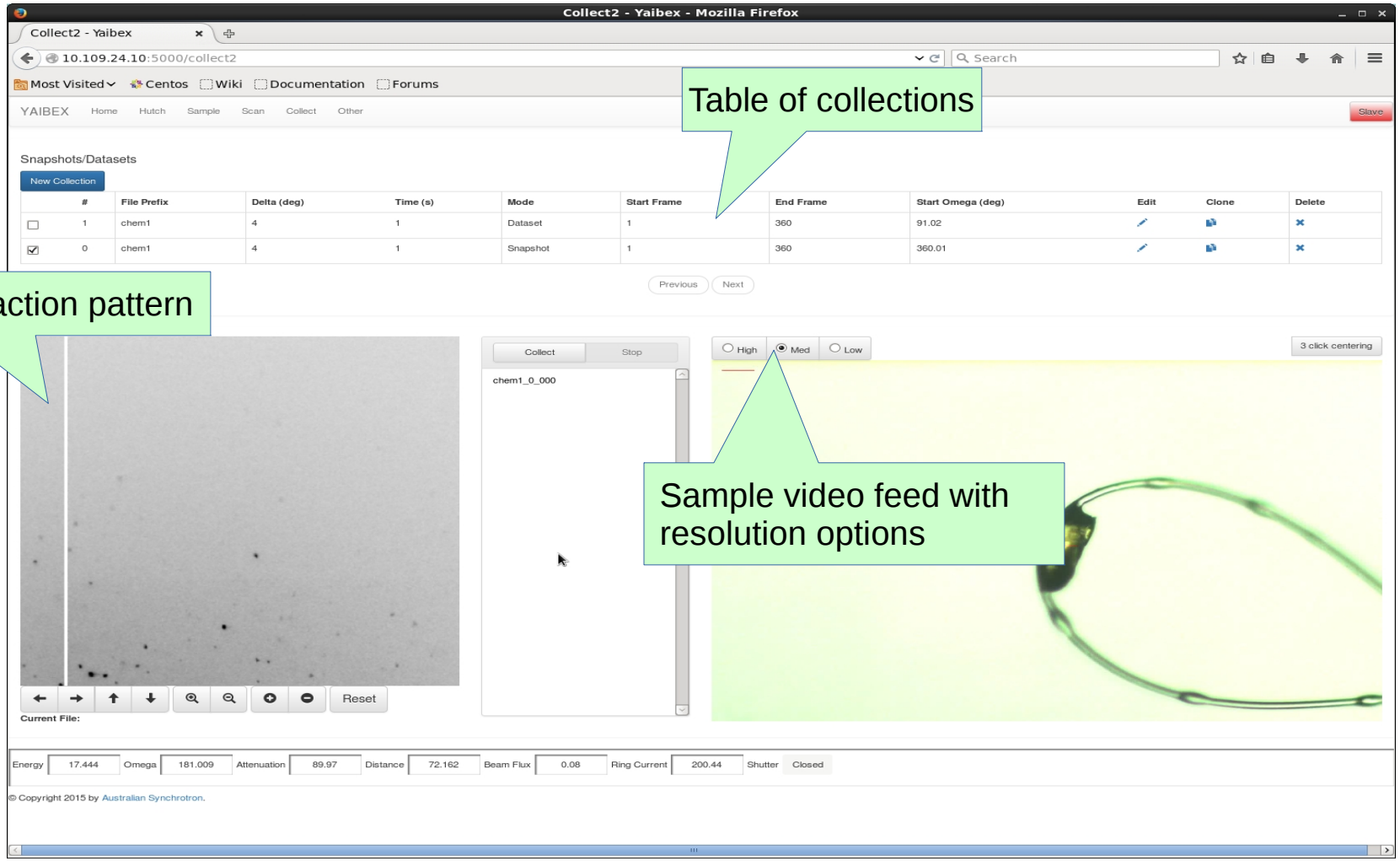

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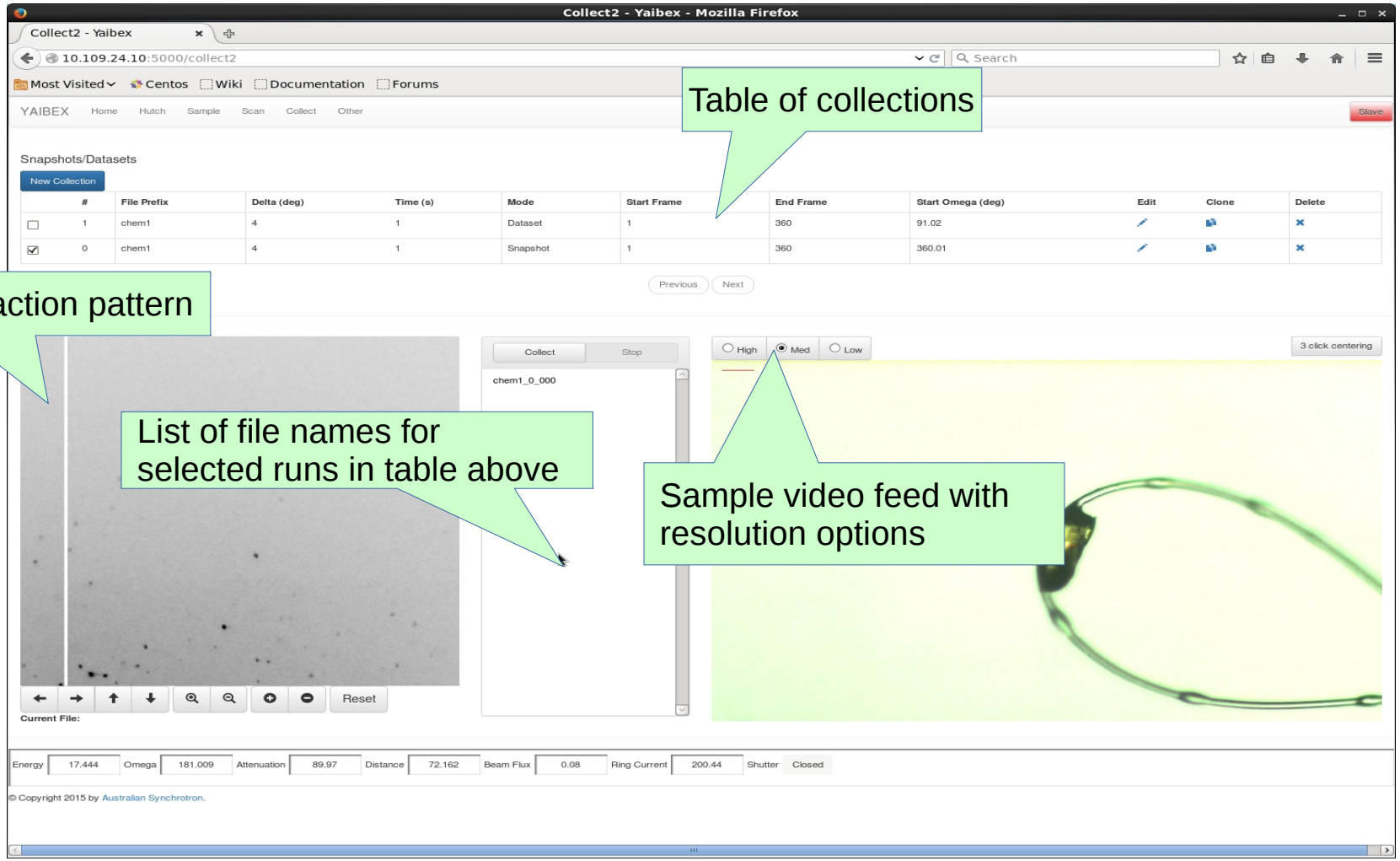

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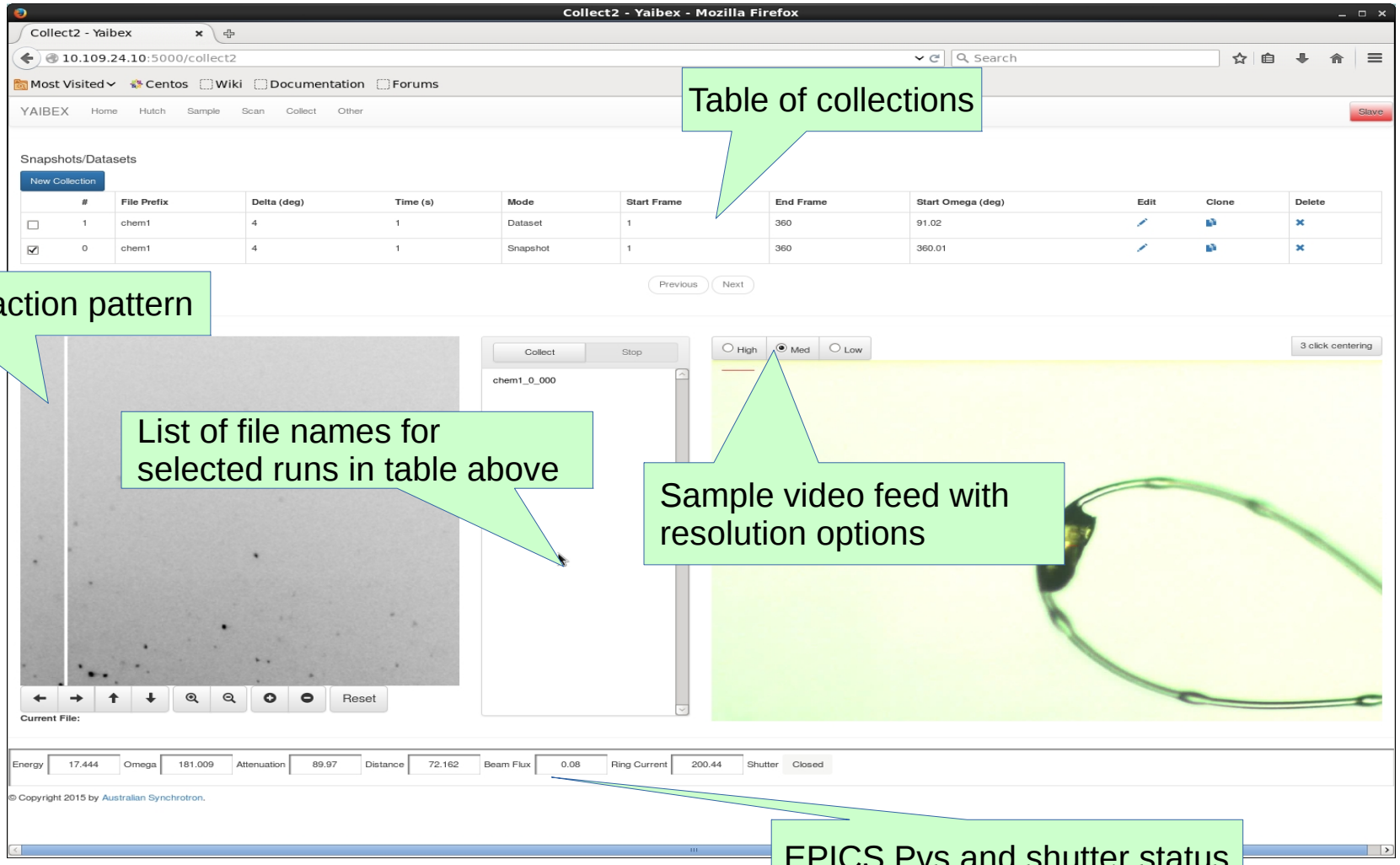

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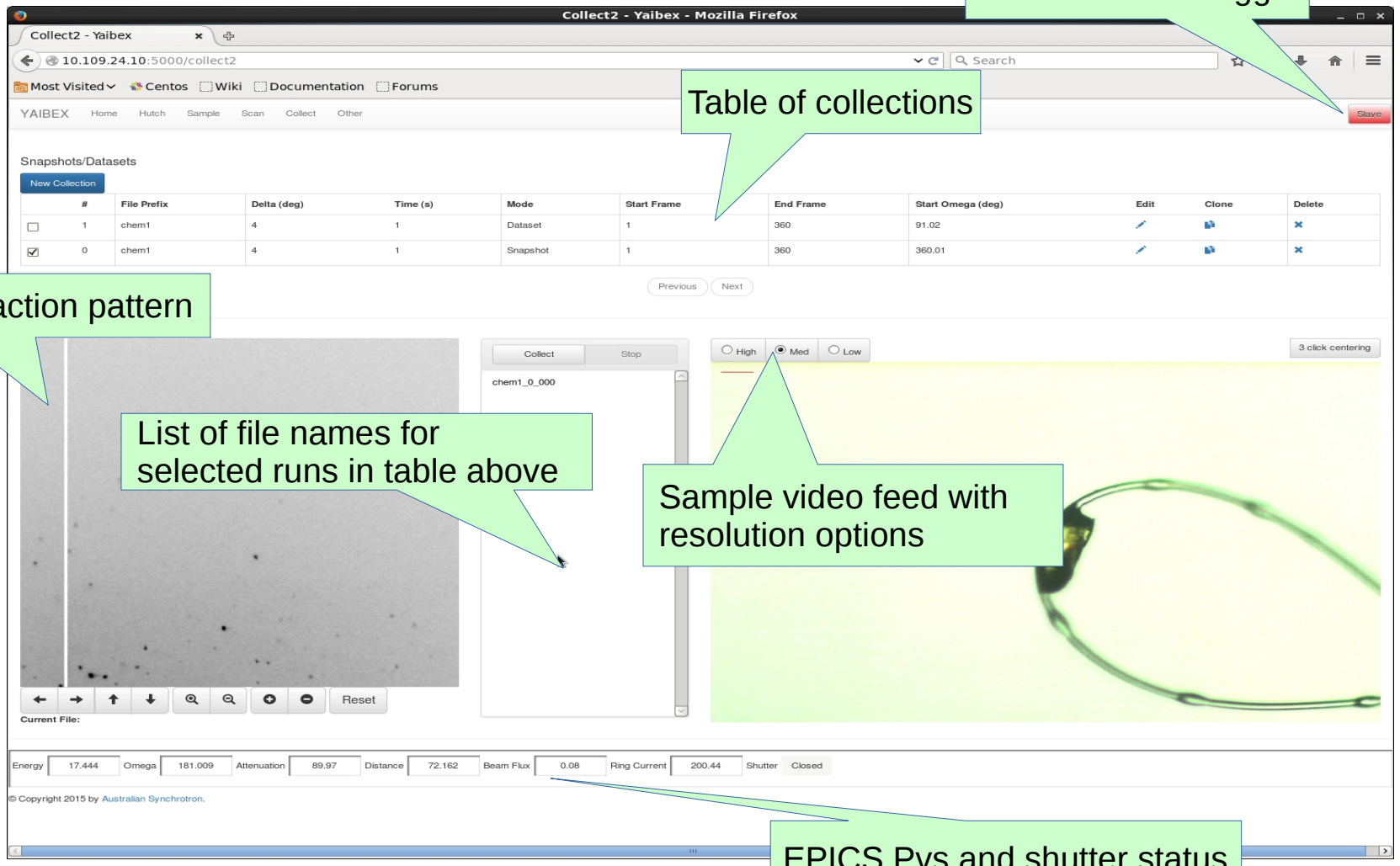

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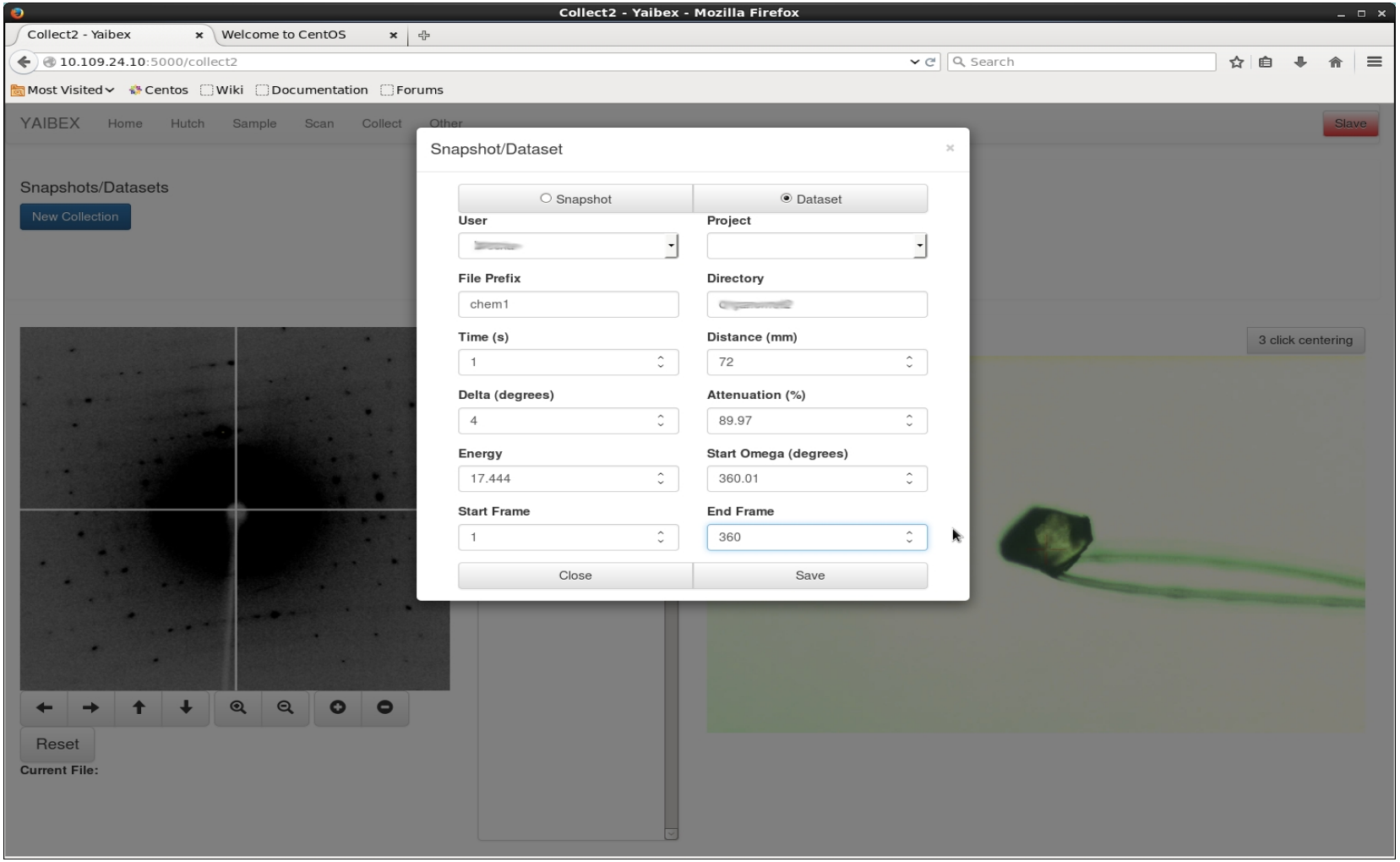

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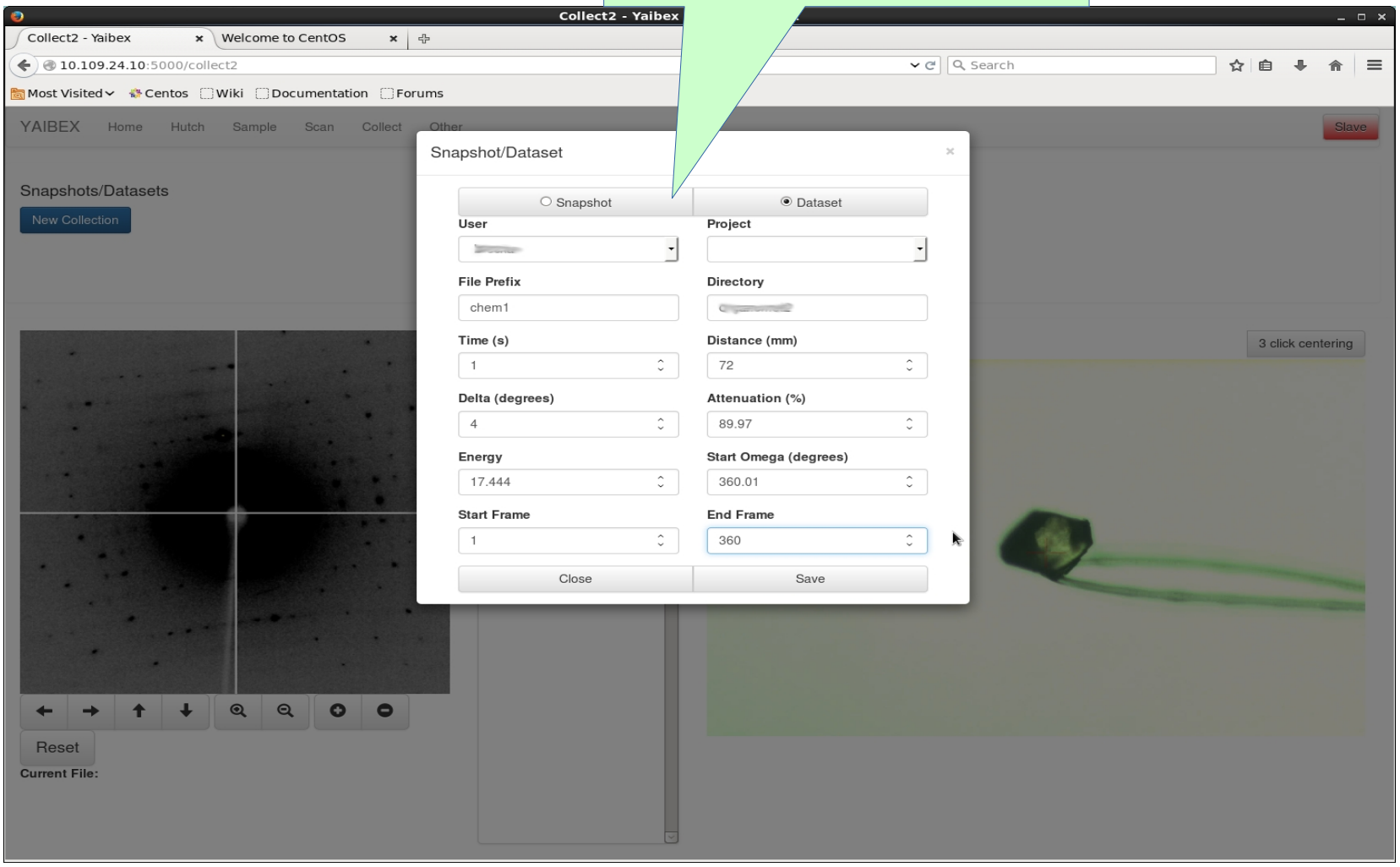

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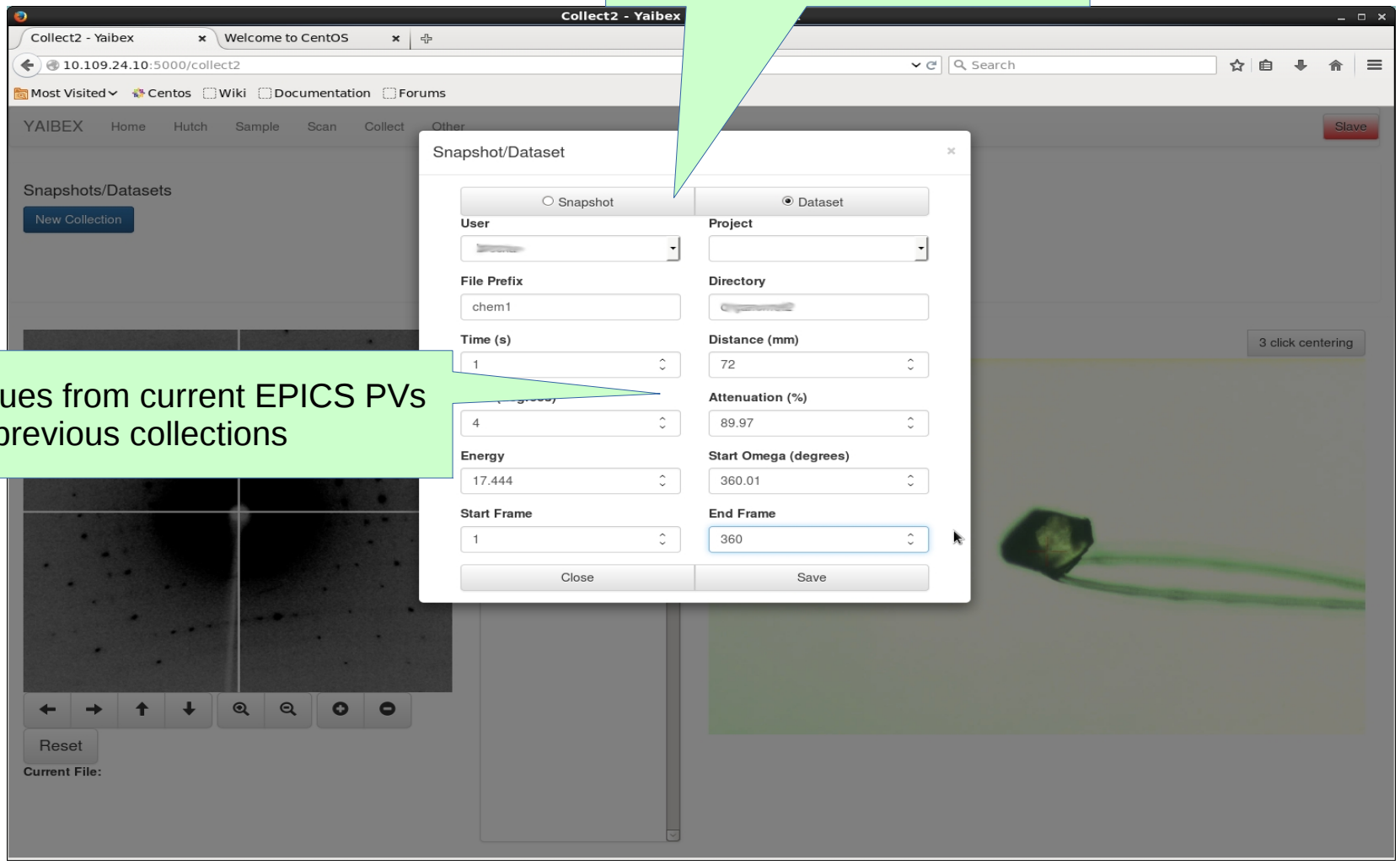

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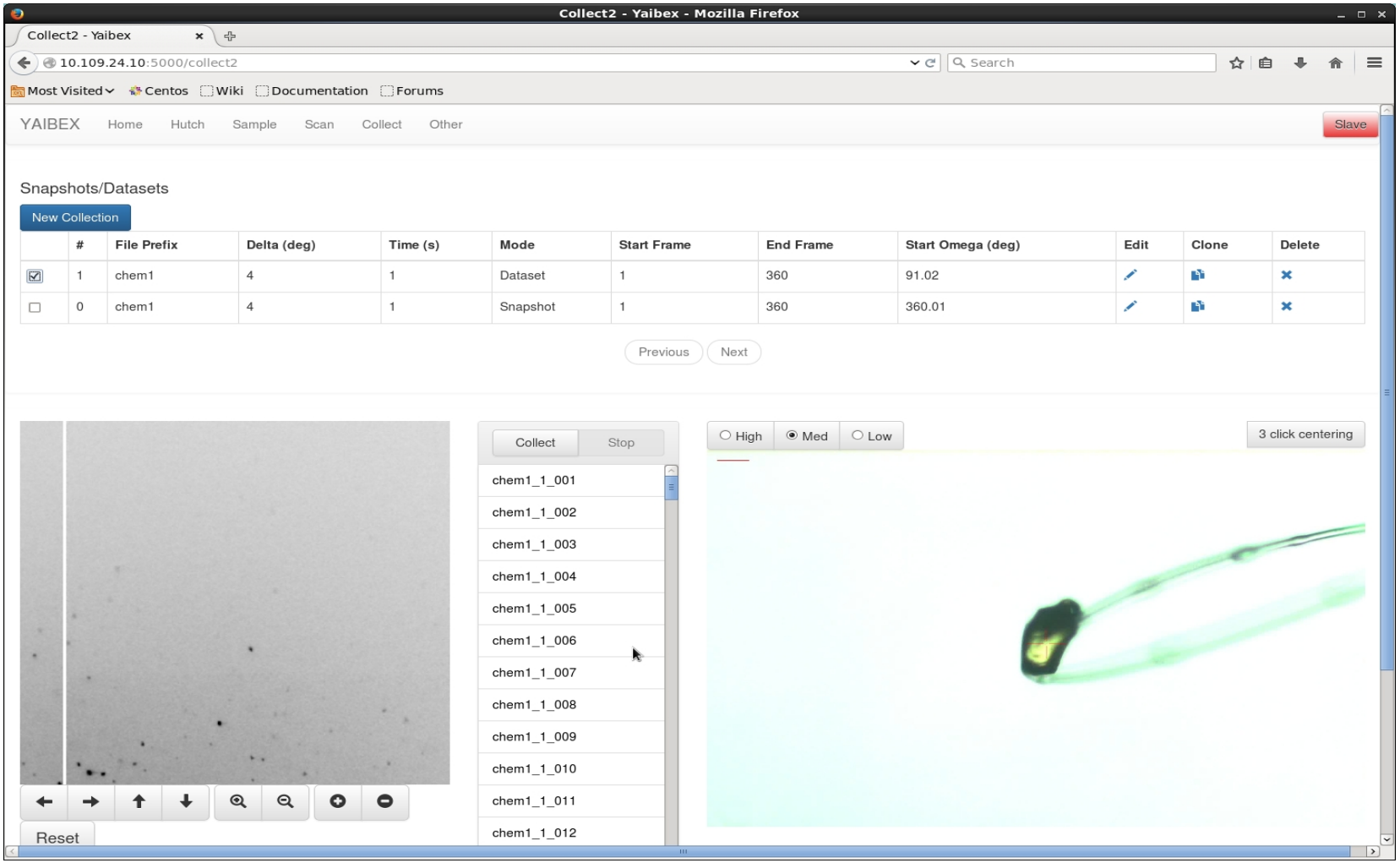

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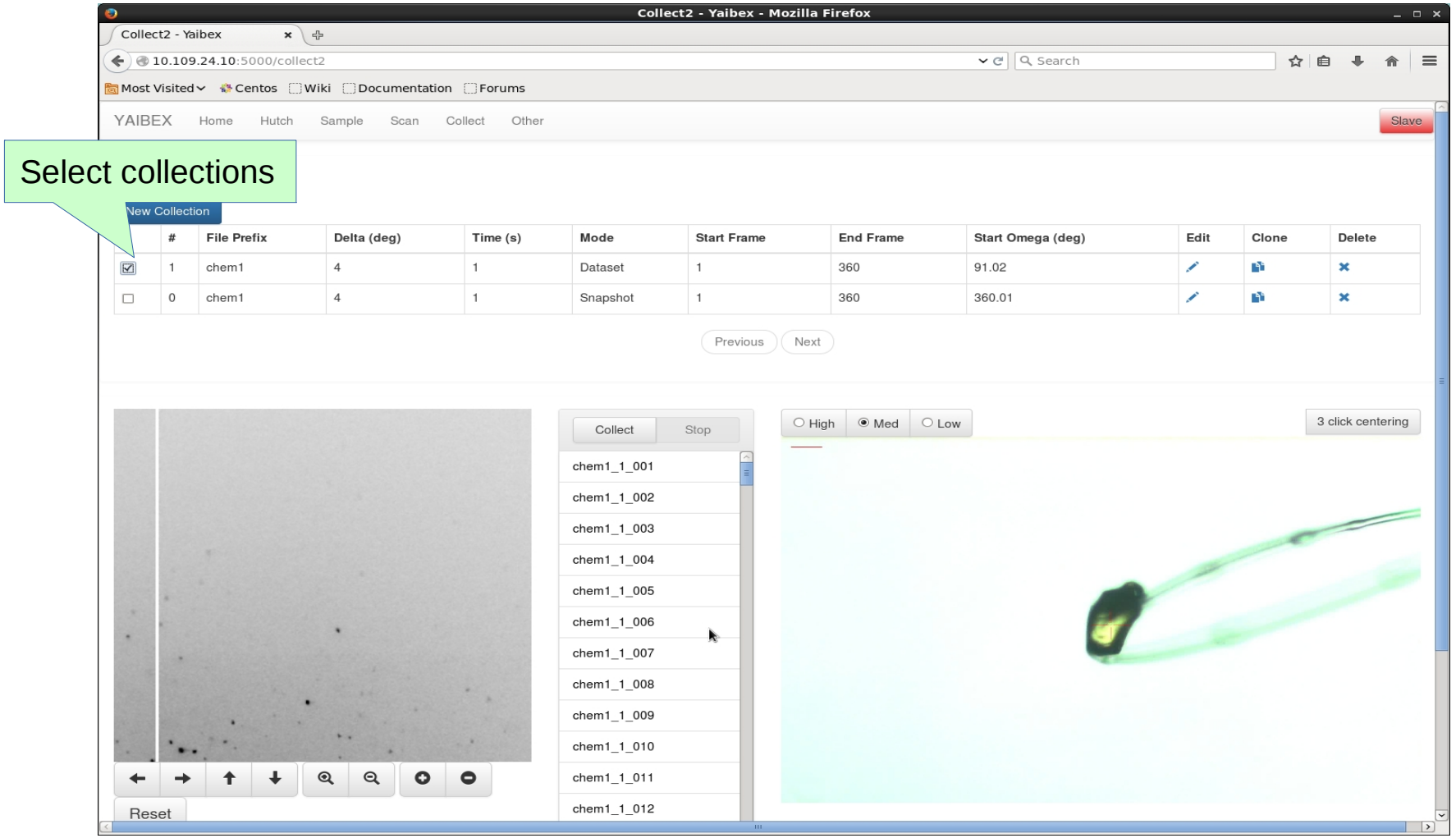

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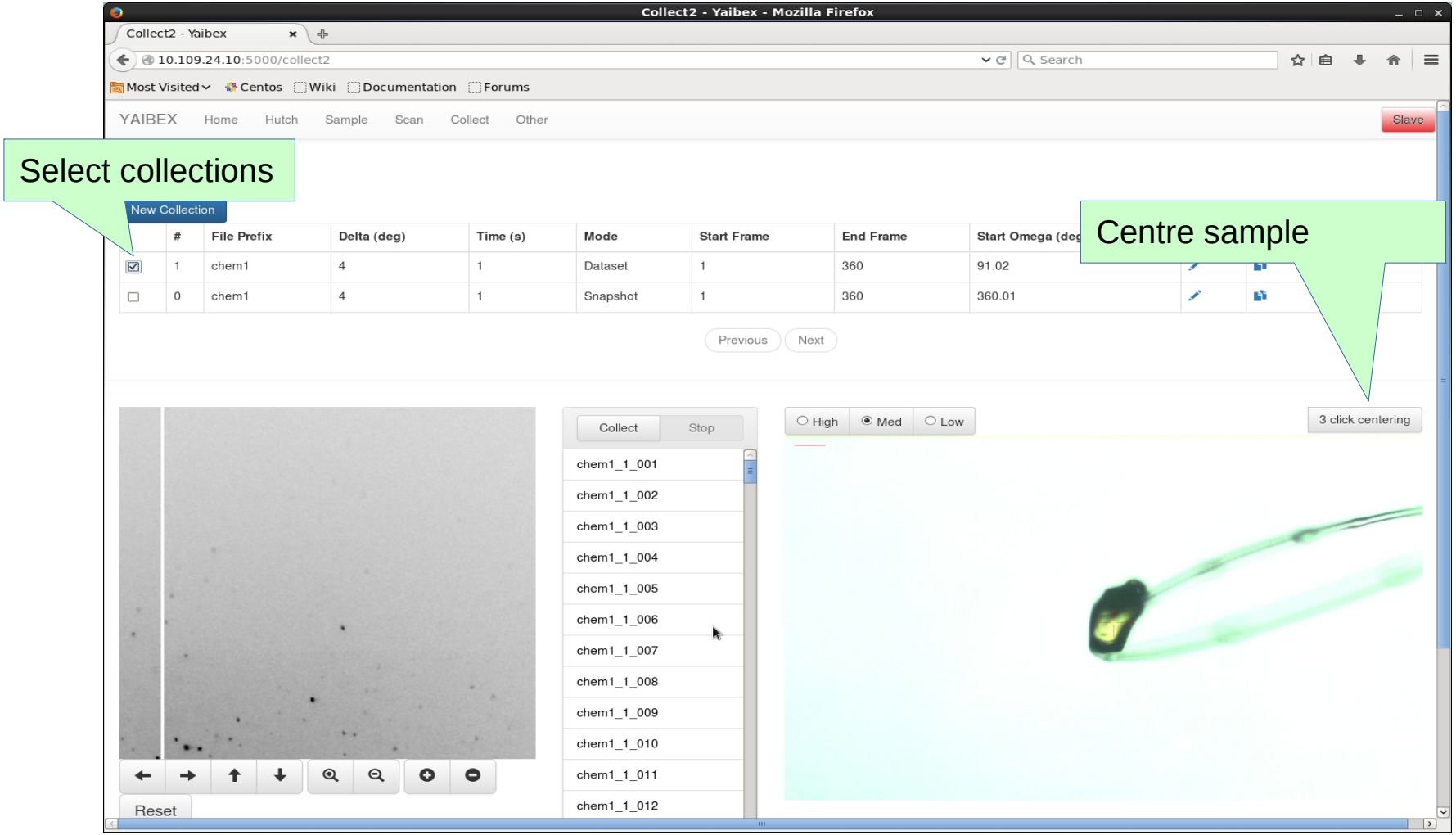

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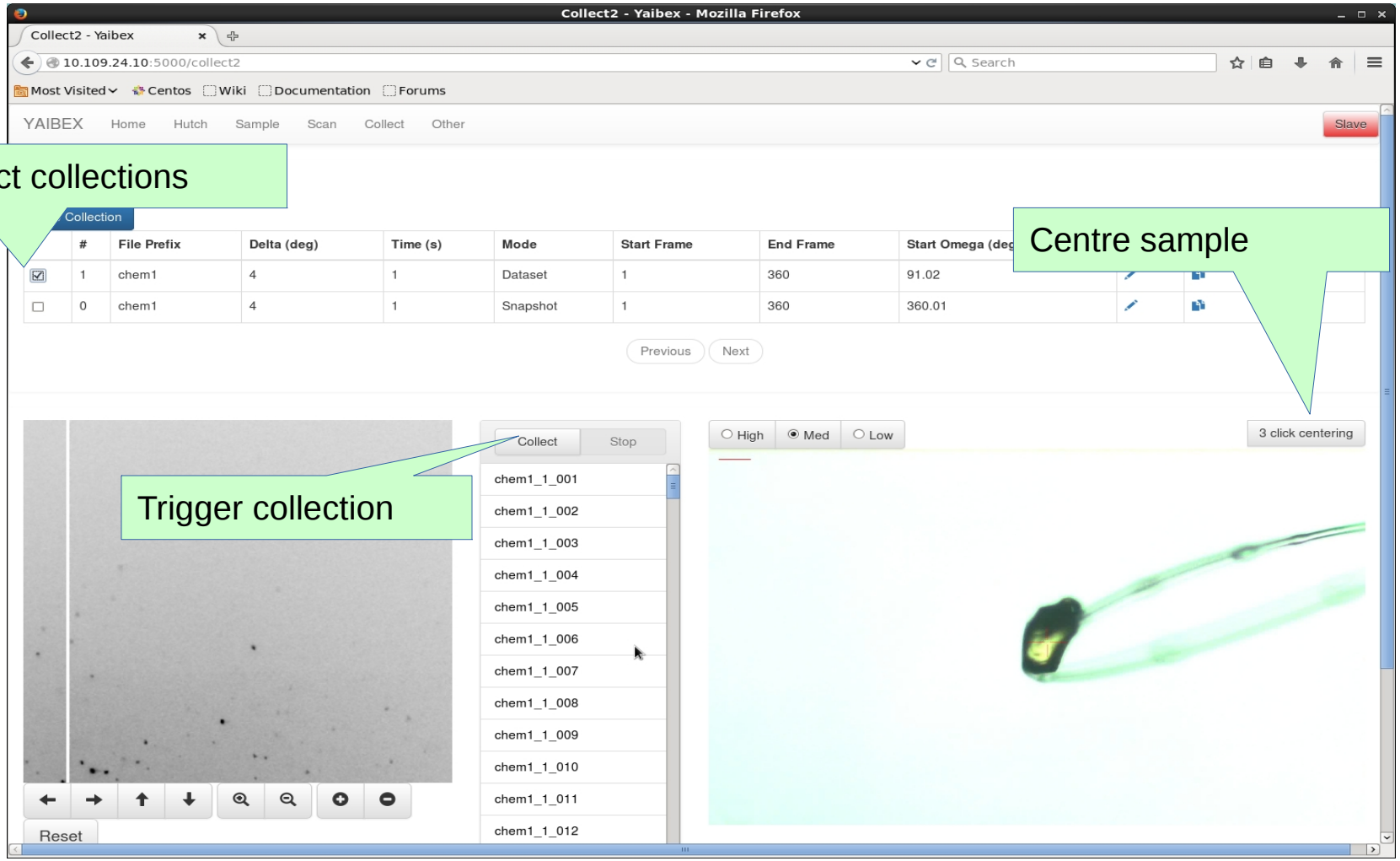

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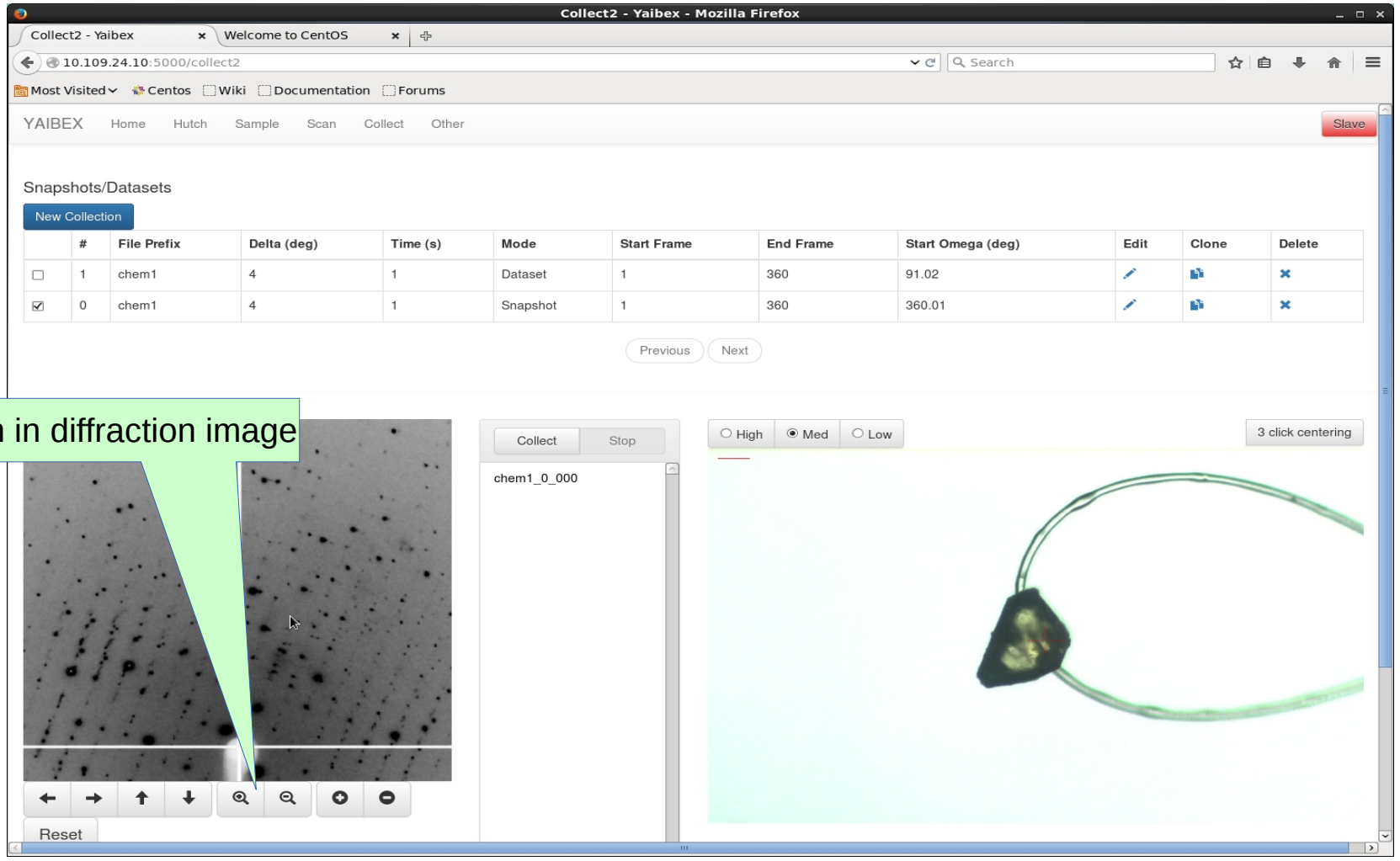

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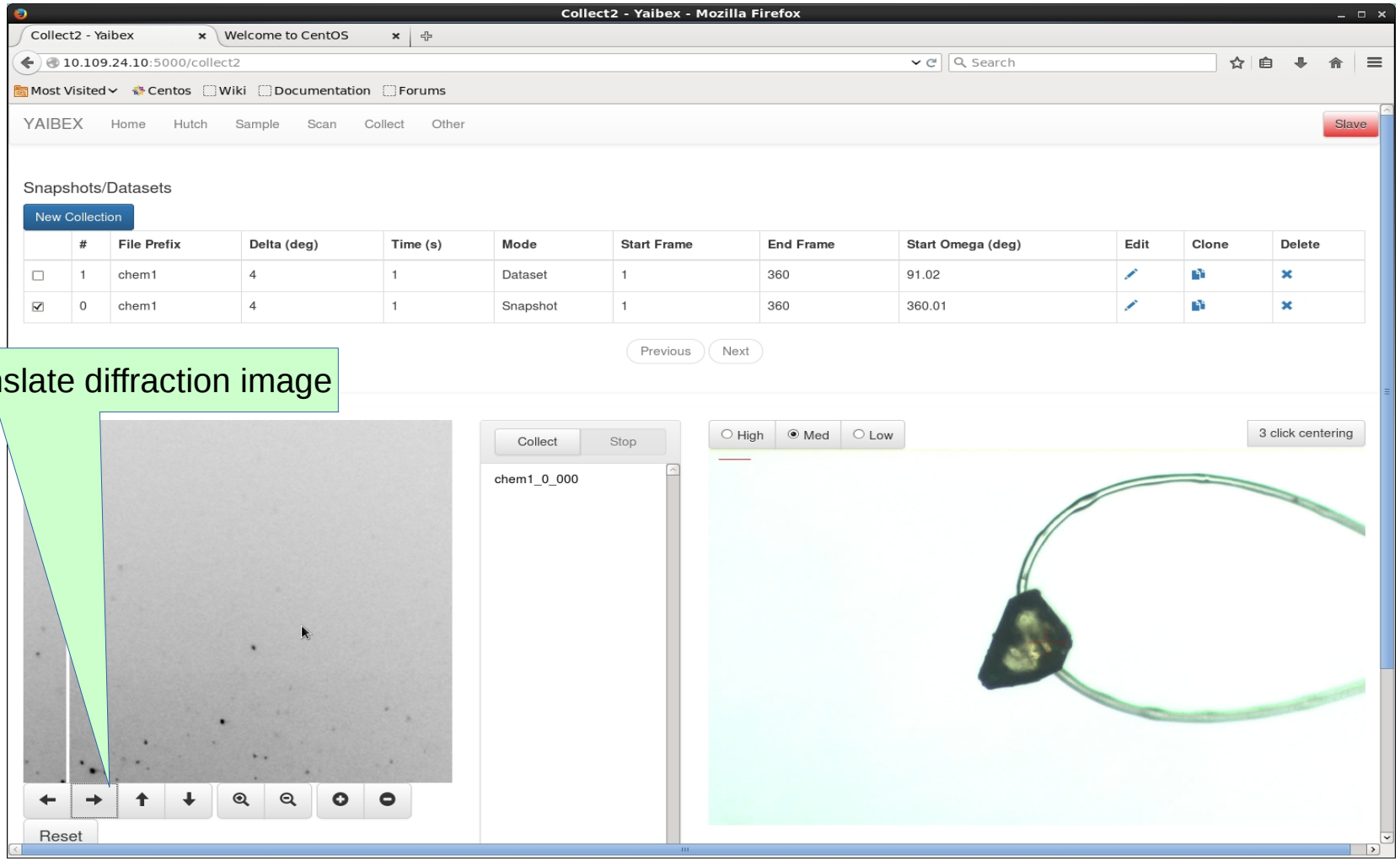

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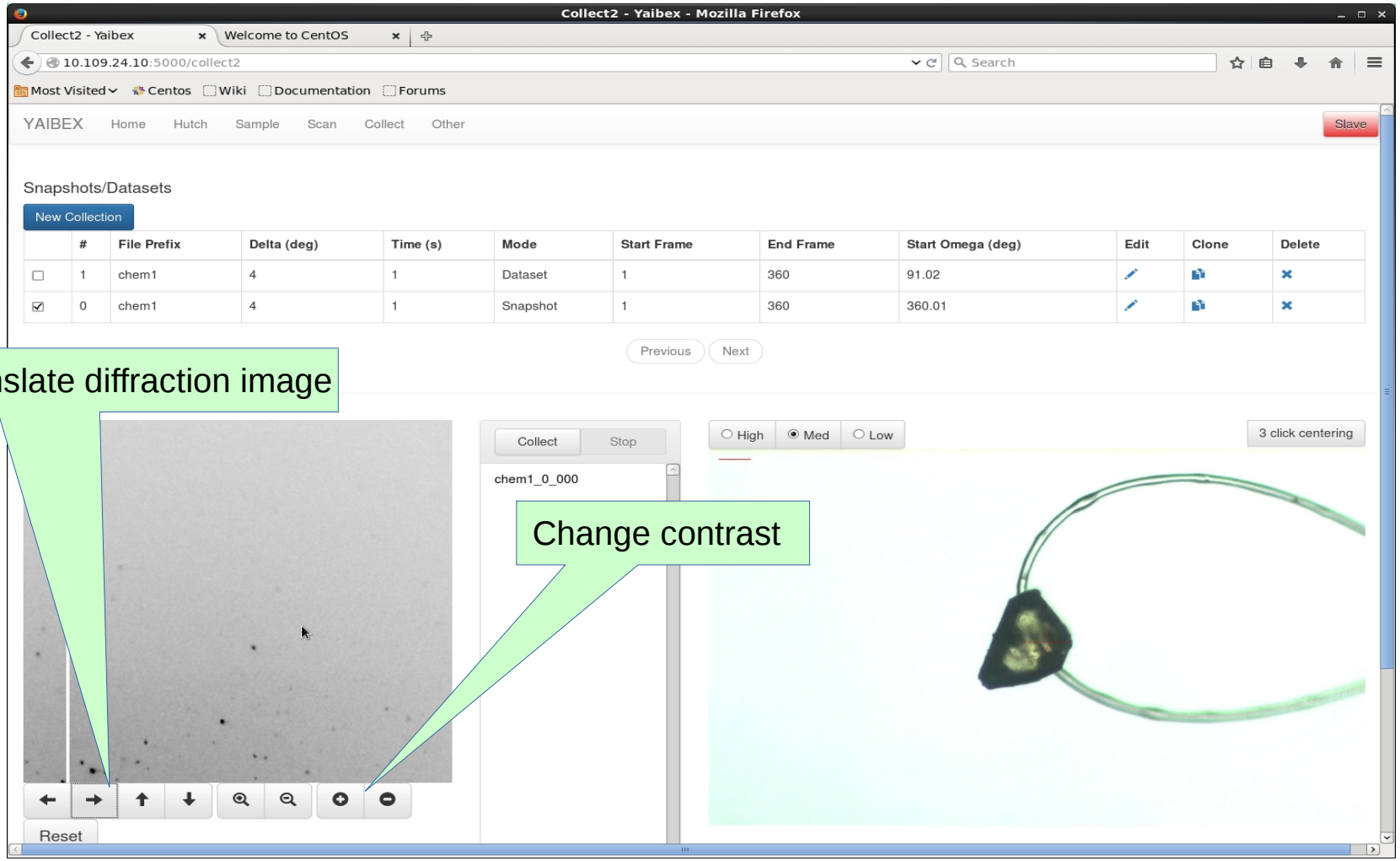


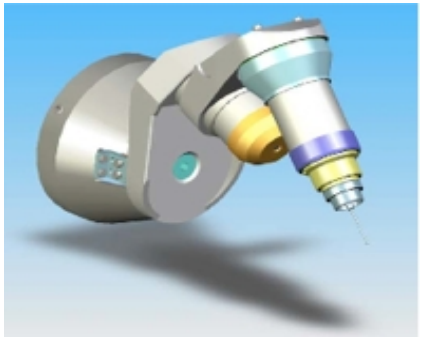
FUNCTIONALITY SUMMARY

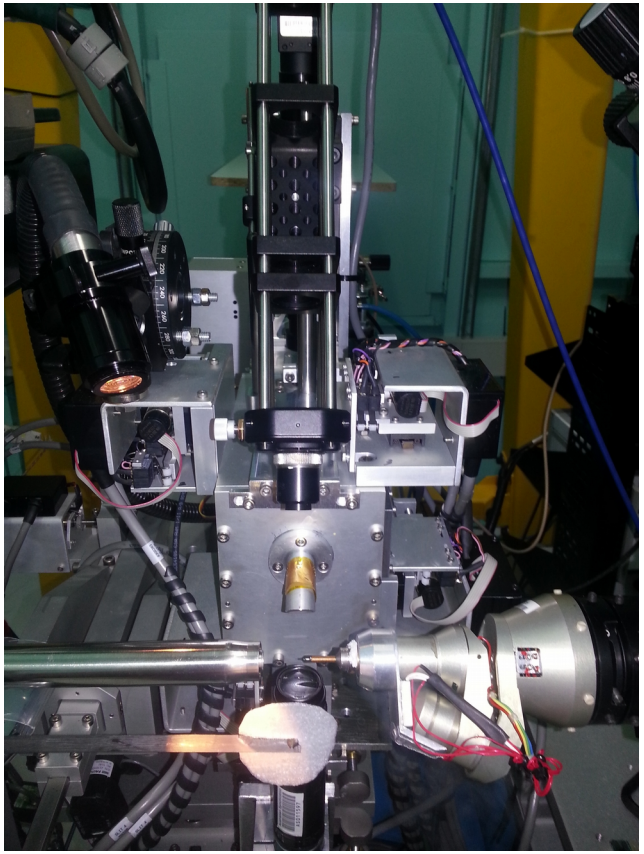
Current:

- Specify data collection parameters for both a single shot and a continuous data set
- Trigger the data collection with reporting of when the shutter is open or shut
- View live feed on sample camera ROI with click-to-centre functionality
- View epics PV values (motor values, beam current etc).
- Integrates with the current Blu-Ice instances so that only one instance can take control of the beamline, and allow switching between active and passive mode
- View the current diffraction pattern, with options to change zoom, translation and contrast.
- Integrates with autoprocessing triggering
- UI designed to work remotely on smaller laptop or tablets

FUTURE DEVELOPMENTS

- Deploy on MX2
- Other "tabs" such as hutch/sample/scan
- Integration with user portal API to fetch user, project and other information.
- Mini kappa





THANKS AND ACKNOWLEDGEMENTS

Thanks to both the SC&IT and MX teams:

David Aragao for driving the project and working with me down at the beamline.

Nathan Mudie for developing a lot of the beamline computing infrastructure YAIBEX uses.

MX beamline staff who have helped with testing and debugging.