# Accessing HB2A data

HB2A Instrument Team

High Flux Isotope Reactor

November 2019

ORNL is managed by UT-Battelle, LLC for the US Department of Energy

# Quick Guide Contents

- **Downloading your Autoreduced Data from ONCat**

- **Accessing the Analysis Cluster**

- **Manual Data Reduction, Plotting and Saving with Mantid**
  - **Finding your data on the Analysis cluster**
  - **Plot diffraction pattern**
  - **Plotting Individual Detectors (e.g. Order Parameter Plots)**
  - **Saving your manually reduced data**

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# Quick Links

- All data is autoreduced and can be downloaded through ONCat: https://oncat.ornl.gov/#/

- Scan run numbers, title, etc are also viewable through ONCat.

- Manual viewing, plotting, reduction and saving of your data with Mantid can be done at **https://analysis.sns.gov/**

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# How To View Scan Details and Download Autoreduced Data

- Every completed scan is autoreduced and accessible through ONCat



https://oncat.ornl.gov/#/
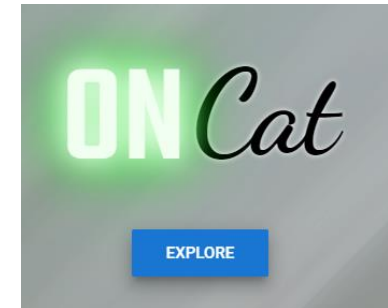
# Steps to access your data from ONCat

1) Login to the system using your unique 3-character code and password

**2) Click on HFIR**

Facilities

HFIR — High Flux Isotope Reactor

SNS — Spallation Neutron Source

ONCat EXPLORE → HFIR

Instruments

| | | |
|---|---|---|
| CG1B | DEV BEAM | Instrument Development Beam Line |
| CG1D | IMAGING | Neutron Imaging Facility |
| CG2 | GP-SANS | General-Purpose Small-Angle Neutron Scattering Diffractometer |
| CG3 | BIO-SANS | Biological Small-Angle Neutron Scattering Instrument |
| CG4C | CTAX | Cold Neutron Triple-Axis Spectrometer |
| HB1 | PTAX | Polarized Triple-Axis Spectrometer |
| HB1A | FIE-TAX | Fixed-Incident-Energy Triple-Axis Spectrometer |
| HB2A | POWDER | Neutron Powder Diffractometer |
| HB2B | NRSF2 | Neutron Residual Stress Mapping Facility |
| HB2C | WAND2 | Wide-Angle Neutron Diffractometer |

https://oncat.ornl.gov/#/explore/HFIR/HB2A
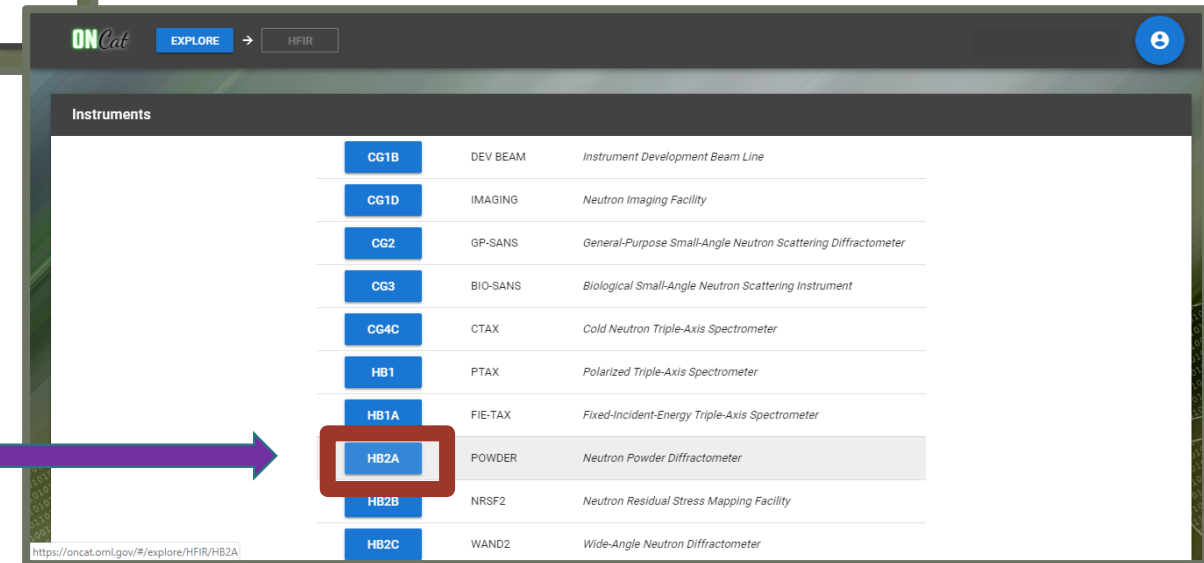
**3) Click on HB2A**

**4) There will be a list of all experiments ran on HB-2A. Click on the IPTS you want to access.**

**NOTE: you can also select the experiment number, but downloading this folder will NOT include autoreduced data, so this is not recommended.**
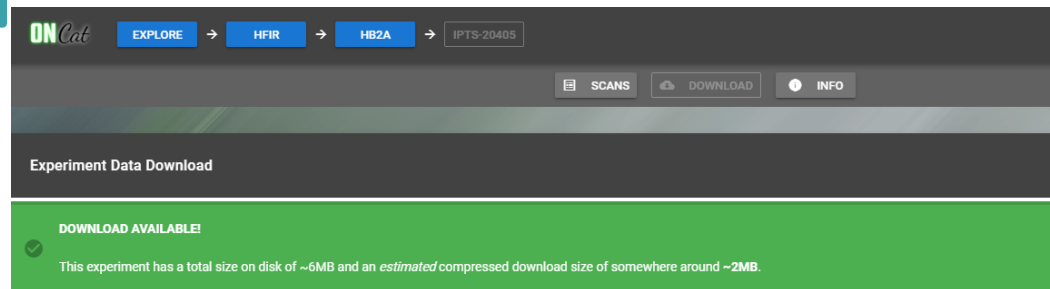
ONCat EXPLORE → HFIR → HB2A

Ragos, Jaime

EXPERIMENTS    SCANS

Experiments

IPTS, Exp, Title or PI

| IPTS | Exp(s) | Title | PI | From | To | Datafiles |
|---|---|---|---|---|---|---|
| IPTS-20405 | EXP624 | Magnetic structure of a pyrochlore osmate | Stuart Calder | 2013/10/17 | 2018/02/26 | 29 |

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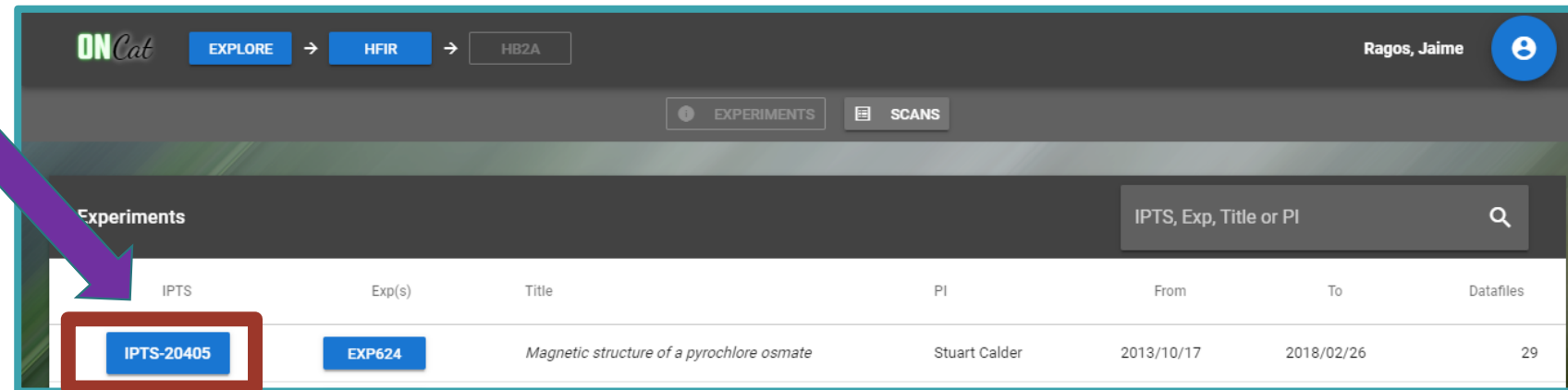
# A Listing of All the Scans Performed is shown



This is where you will find the command used on the scan

This is where you will find the scan title

This is where you will find the Scan number

This shows where the data is located on the analysis clusters (see later)

| Completed | Command | Title | Scan # | Sample Name | Path |
|---|---|---|---|---|---|
| 2018/02/26 10:56:36 EST | scan 2theta 8 14 0.05 preset time 60 | Hg2Os2O7, Ge115 (1.54A), op-21-12. T=110 K | 23 | Hg2Os2O7 | /HFIR/HB2A/IPTS-20405/exp624/Datafiles/HB2A_exp0624_scan0023.dat |
| 2018/02/26 08:51:11 EST | scan 2theta 8 14 0.05 preset time 60 | Hg2Os2O7, Ge115 (1.54A), op-21-12. T=110 K | 22 | Hg2Os2O7 | /HFIR/HB2A/IPTS-20405/exp624/Datafiles/HB2A_exp0624_scan0022.dat |
| 2018/02/26 06:45:51 EST | scan 2theta 8 14 0.05 preset time 60 | Hg2Os2O7, Ge115 (1.54A), op-21-12. T=110 K | 21 | Hg2Os2O7 | /HFIR/HB2A/IPTS-20405/exp624/Datafiles/HB2A_exp0624_scan0021.dat |
| 2018/02/26 04:25:33 EST | scan 2theta 8 14 0.05 preset time 60 | Hg2Os2O7, Ge115 (1.54A), op-21-12. T=25 K | 20 | Hg2Os2O7 | /HFIR/HB2A/IPTS-20405/exp624/Datafiles/HB2A_exp0624_scan0020.dat |
| 2018/02/26 02:20:26 EST | scan 2theta 8 14 0.05 preset time 60 | Hg2Os2O7, Ge115 (1.54A), op-21-12. T=25 K | 19 | Hg2Os2O7 | /HFIR/HB2A/IPTS-20405/exp624/Datafiles/HB2A_exp0624_scan0019.dat |
| 2018/02/26 00:15:26 EST | scan 2theta 8 14 0.05 preset time 60 | Hg2Os2O7, Ge115 (1.54A), op-21-12. T=25 K | 18 | Hg2Os2O7 | /HFIR/HB2A/IPTS-20405/exp624/Datafiles/HB2A_exp0624_scan0018.dat |
| 2018/02/25 22:10:29 EST | scan 2theta 8 14 0.05 preset time 60 | Hg2Os2O7, Ge115 (1.54A), op-21-12. T=25 K | 17 | Hg2Os2O7 | /HFIR/HB2A/IPTS-20405/exp624/Datafiles/HB2A_exp0624_scan0017.dat |
| 2018/02/25 20:05:34 EST | scan 2theta 8 14 0.05 preset time 60 | Hg2Os2O7, Ge115 (1.54A), op-21-12. T=25 K | 16 | Hg2Os2O7 | /HFIR/HB2A/IPTS-20405/exp624/Datafiles/HB2A_exp0624_scan0016.dat |
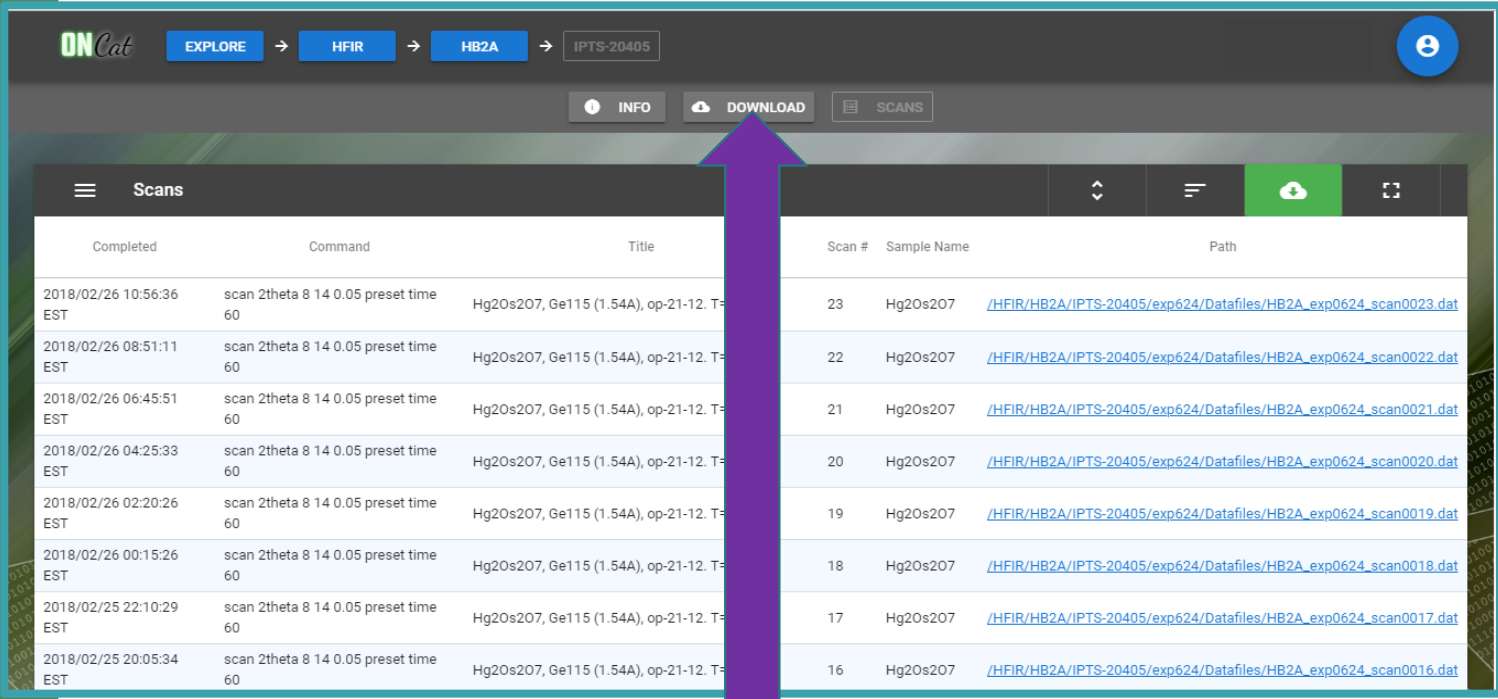
5) Click Download, then "Start Download" on next screen to get your data.
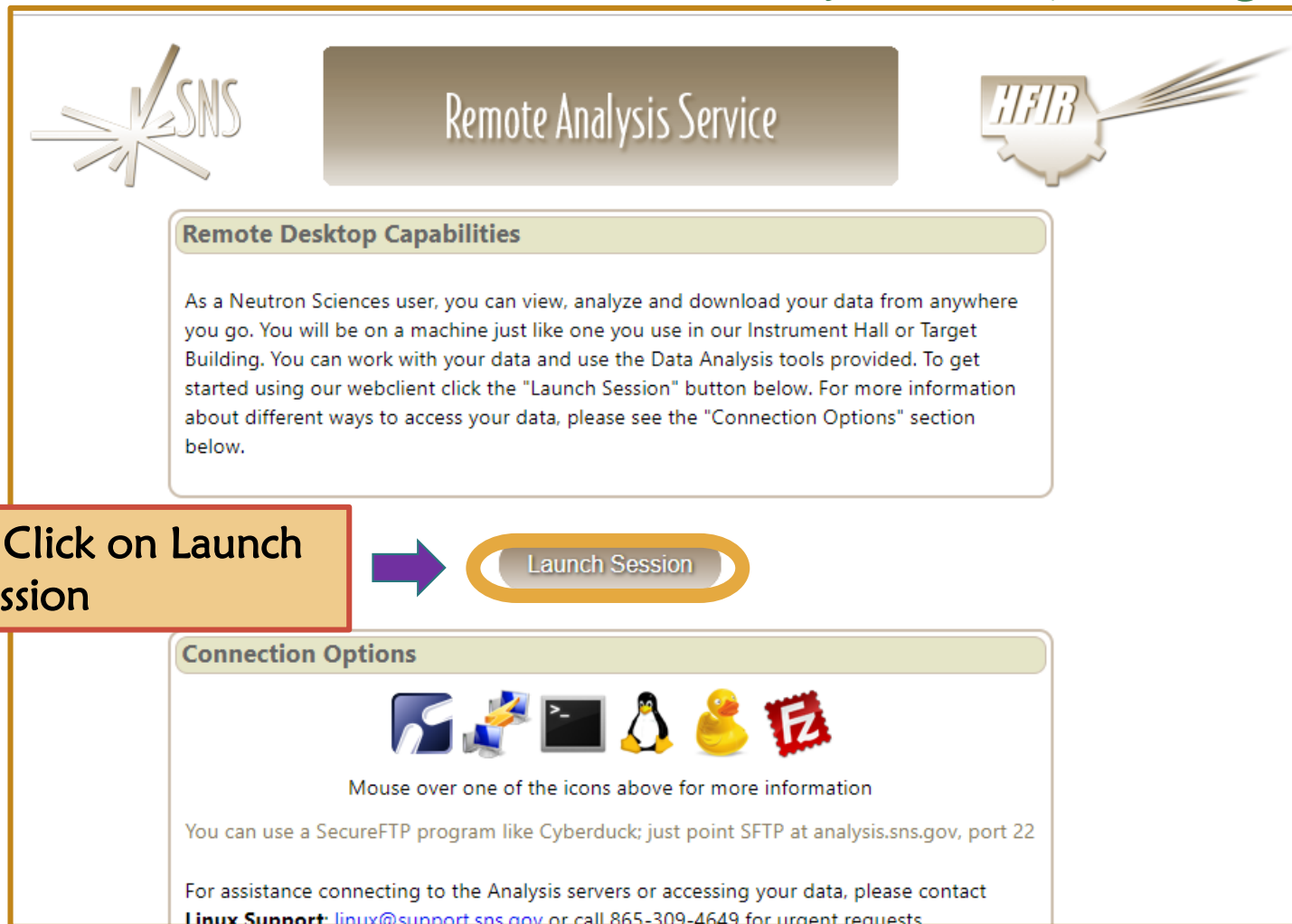Autoreduced data is in:
IPTS-XXXX/shared/autoreduce/

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# Manually View and Save Your Data

- **All scans are autoreduced into a format ready for viewing and refinement.**

- **But** if you need to manually view, plot, reduce, save your data then the following steps show how to do this using Mantid through analysis.sns.gov

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# Accessing the analysis service

Go to https://analysis.sns.gov



1) Click on Launch Session
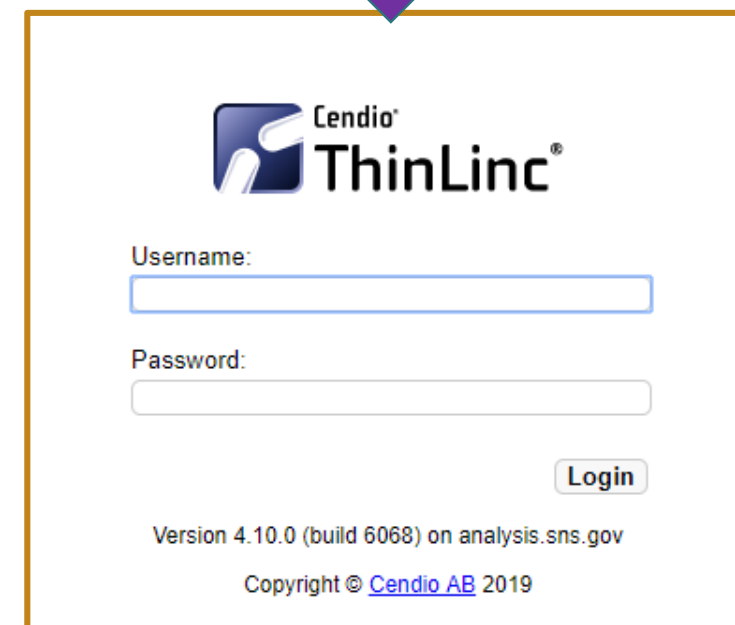
2) You should be redirected to this site where you will need to login with your unique 3-character code and password or your guest username and password
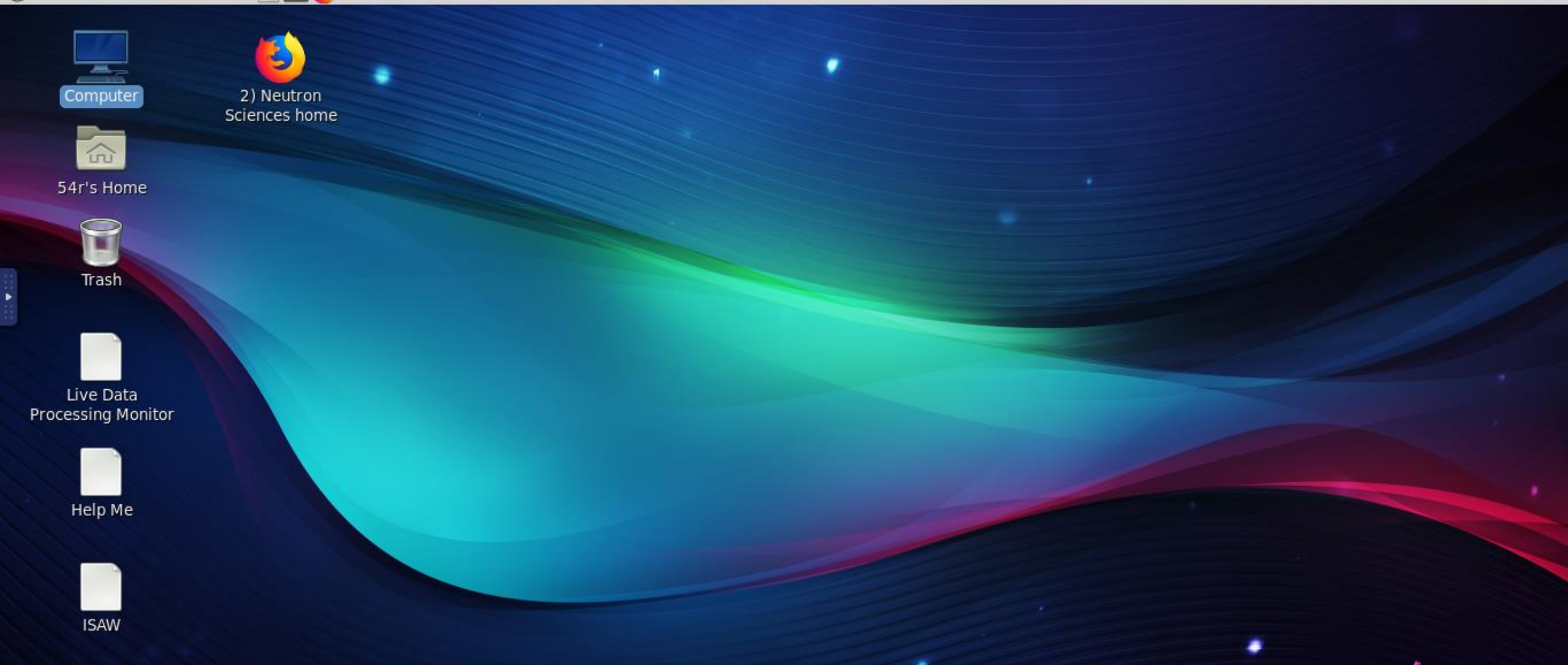
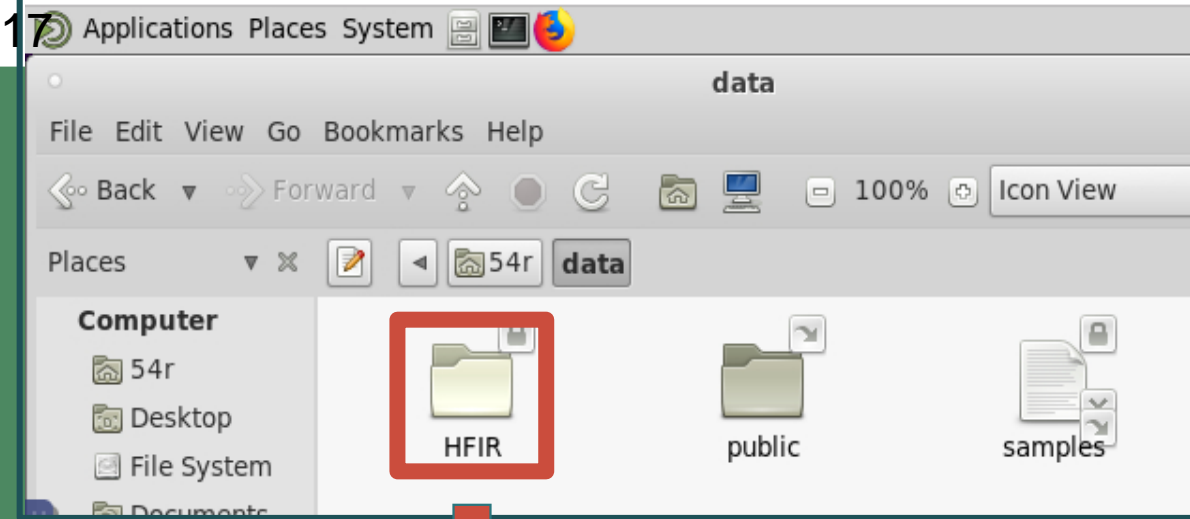3) After logging in a second time you should have a remote desktop open

*Note: After any long period of inactivity you will be asked to login again
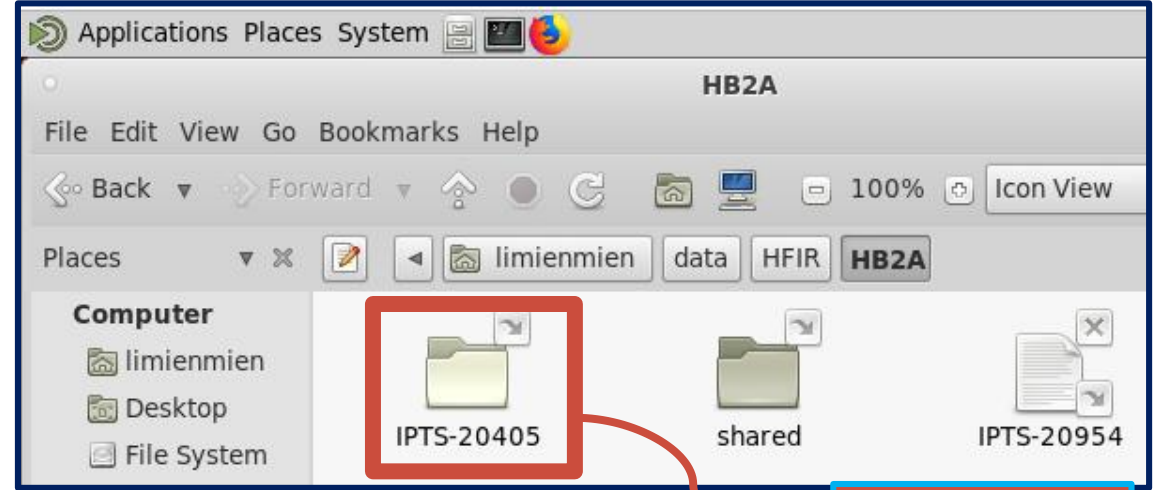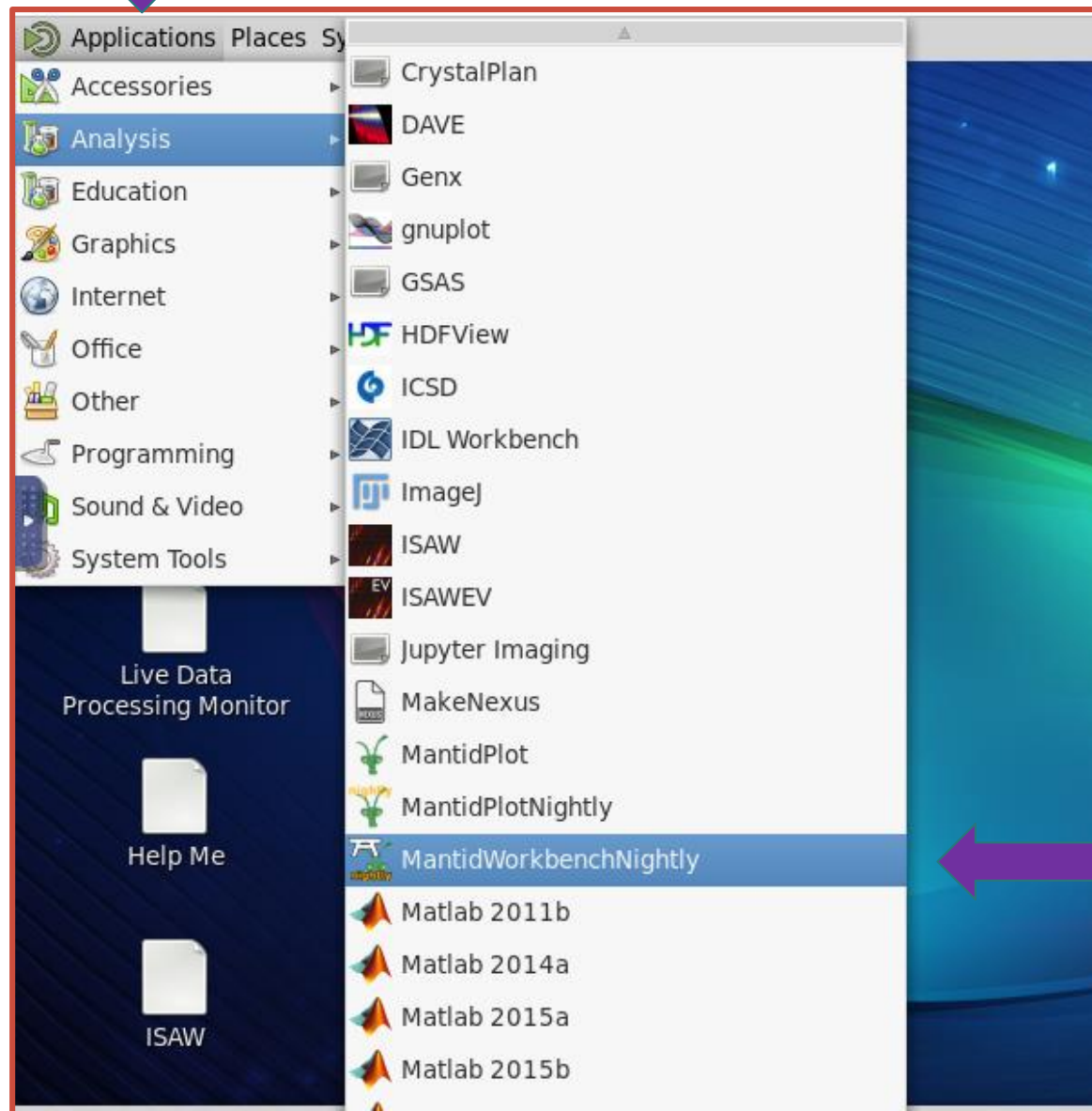
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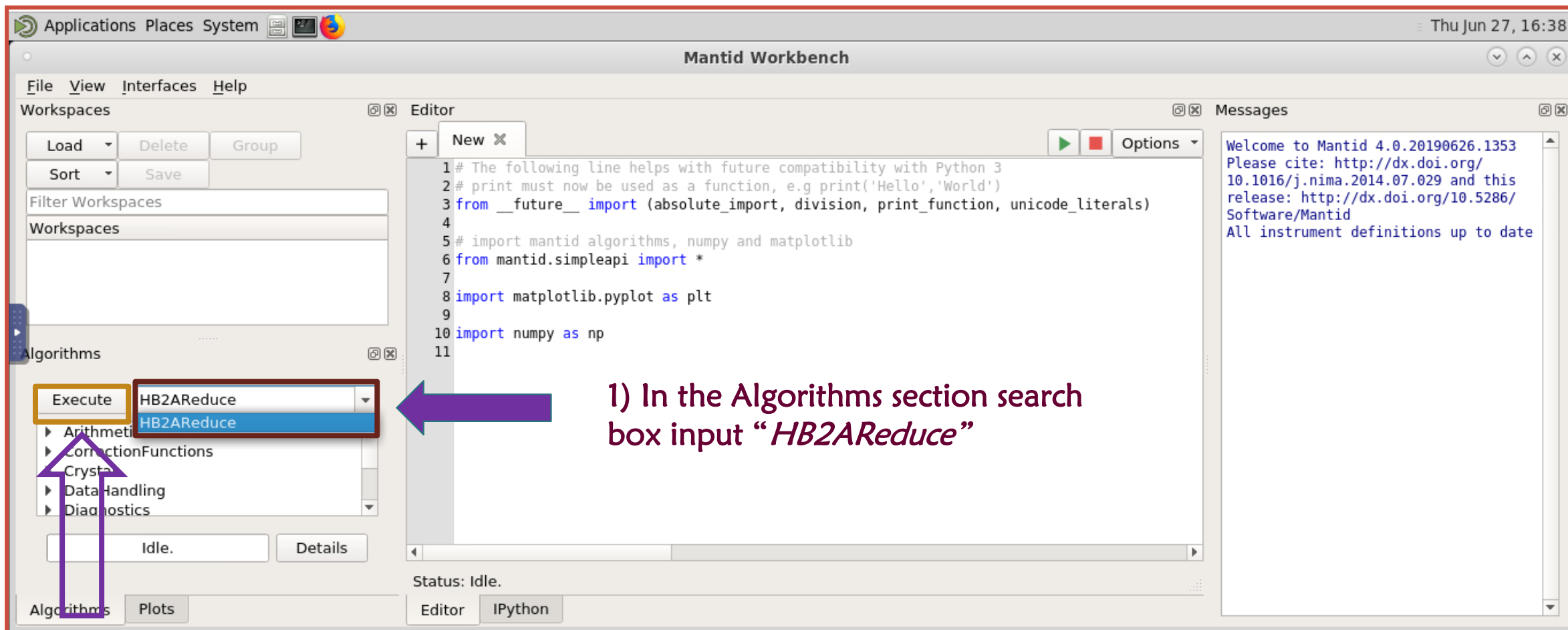  - Saving your manually reduced data

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# Your data is stored on the analysis cluster under your IPTS number



1) Click on your unique file folder

2) Click on Data
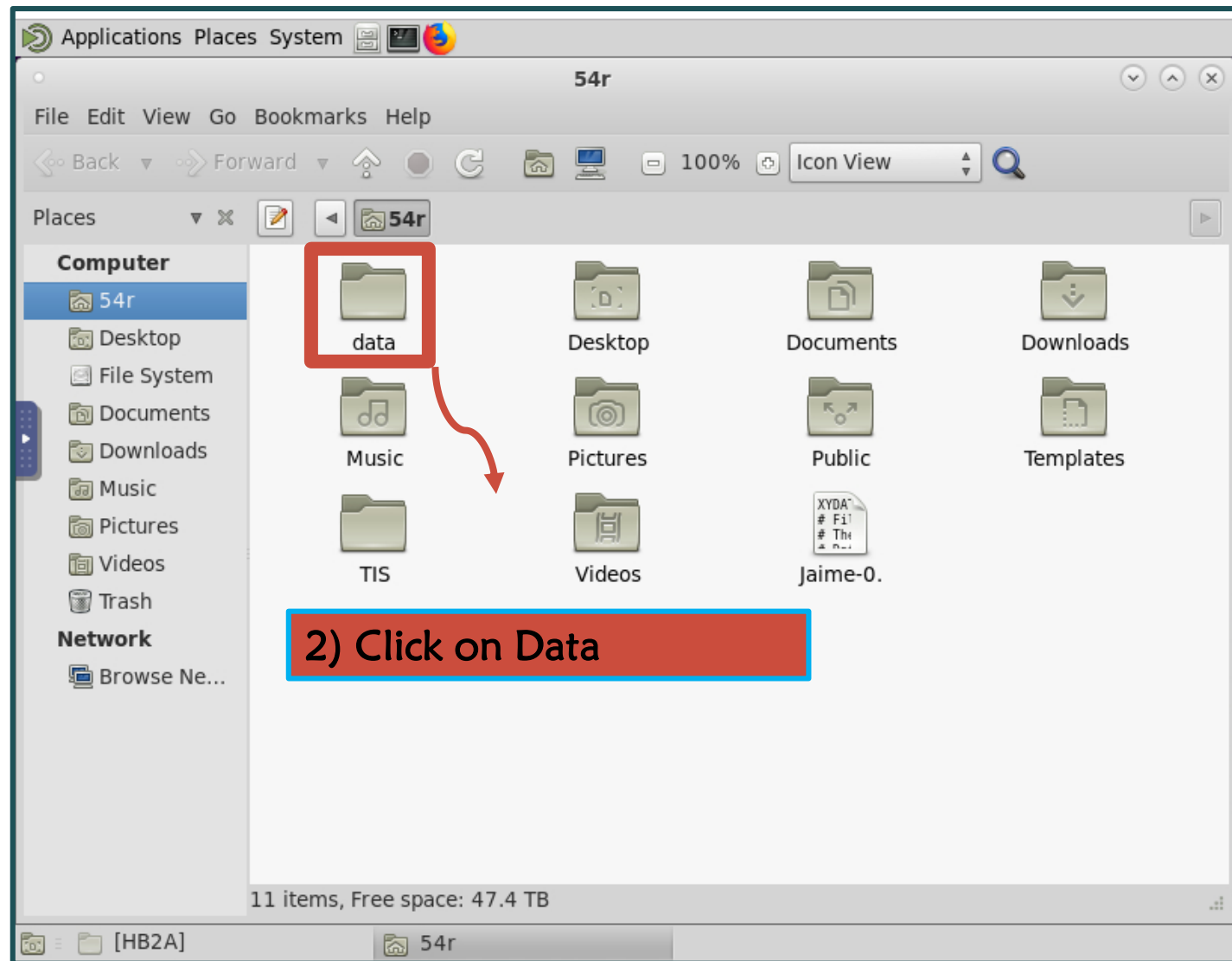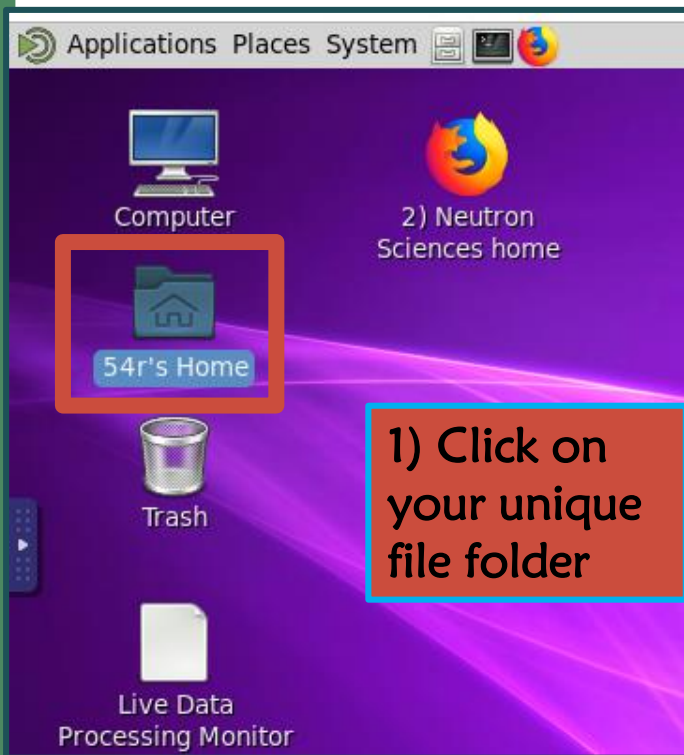
3) Click on HFIR

5) Click on your IPTS
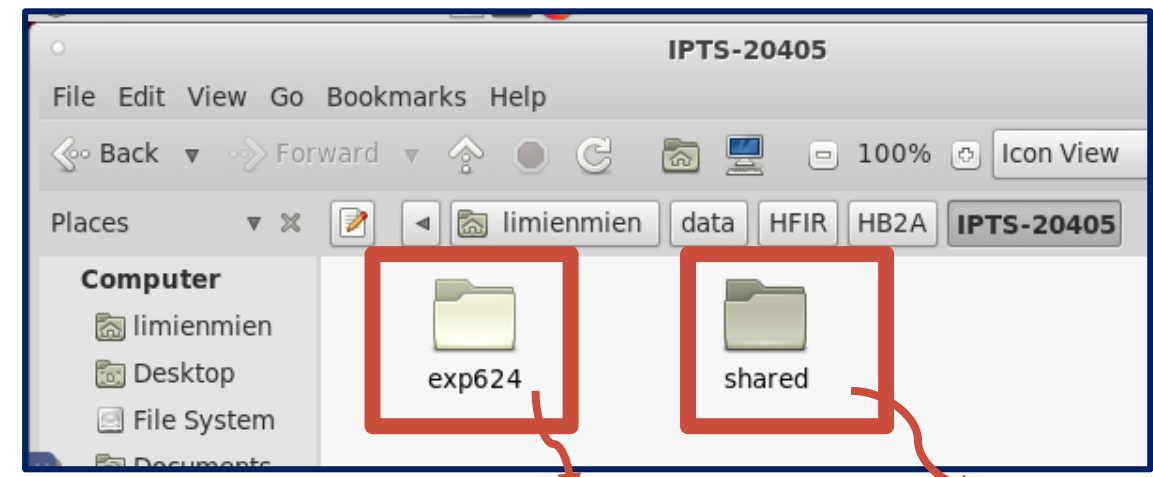
4) Click on HB2A

6) The exp folder contains all the files from the HB2A instrument computer, including raw data, normalization files, excluded detectors, etc.

7) The autoreduced files are stored here.
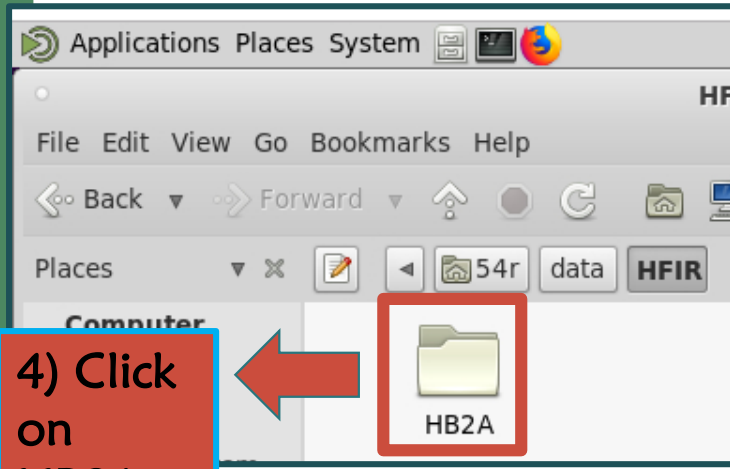
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# Open Mantid

**1) Click on Applications**

**2) Click on Analysis**

**3) Click on MantidWorkbenchNightly**



Applications  Places  Sy

- Accessories ▶
- Analysis ▶
- Education ▶
- Graphics ▶
- Internet ▶
- Office ▶
- Other ▶
- Programming ▶
- Sound & Video ▶
- System Tools ▶

- CrystalPlan
- DAVE
- Genx
- gnuplot
- GSAS
- HDFView
- ICSD
- IDL Workbench
- ImageJ
- ISAW
- ISAWEV
- Jupyter Imaging
- MakeNexus
- MantidPlot
- MantidPlotNightly
- MantidWorkbenchNightly
- Matlab 2011b
- Matlab 2014a
- Matlab 2015a
- Matlab 2015b

Live Data Processing Monitor

Help Me

ISAW

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# Open the HB2AReduce input dialogue window



1) In the Algorithms section search box input "*HB2AReduce*"

2) Click Execute to start the Algorithm

*About Mantid: There are many advanced capabilities in Mantid. The algorithm may be scripted, but we will use the GUI

# HB2AReduce input dialogue window



**Typically leave empty** since we will supply the ScanNumbers
*NOTE: If running Mantid on local computer and not analysis will need to browse for file*

To plot data input IPTS and Exp and put a single or multiple Scan Numbers (e.g. 12,13,14,27 or 12-14,27). *(Scan details can be found using ONCat, see earlier in guide for details)*

**Typically leave empty** to use default vanadium normalization. Check Normalize.

**Typically keep unchecked.** Clicking this box allows you to view each separate detector. *(The section on individual detectors will show what happens if this box is selected)*

BinData: Check this combine detector counts and create diffraction pattern.

Put name to label output workspace file

**Typically leave empty.** Exclude detector only when advised by instrument team, otherwise leave blank

**Typically leave empty and default will be used.** Allows alternative x values to be defined

Define data bin size (0.05 is default)

Define arbitrary scale factor (default is 20000)

This button is FAQ, if you need any additional help click this

If you want this window to stay open after you run the program click this box

Clicking this to run the reduction

HB2AReduce input dialog

Performs data reduction for HB-2A POWDER at HFIR

| Filename | | Browse |
| IPTS | 20405 | |
| Exp | 624 | |
| ScanNumbers | 12 | |
| Vanadium | | Browse |
| | ✓ Normalise | |
| ExcludeDetectors | | |
| DefX | | |
| | ☐ IndividualDetectors | |
| | ✓ BinData | |
| BinWidth | 0.05 | |
| Scale | 20000 | |
| **OutputWorkspace** | Sample 1 | |

?      Keep Open ✓   Run   Close

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# Running HB2AReduce

# Workspace files created
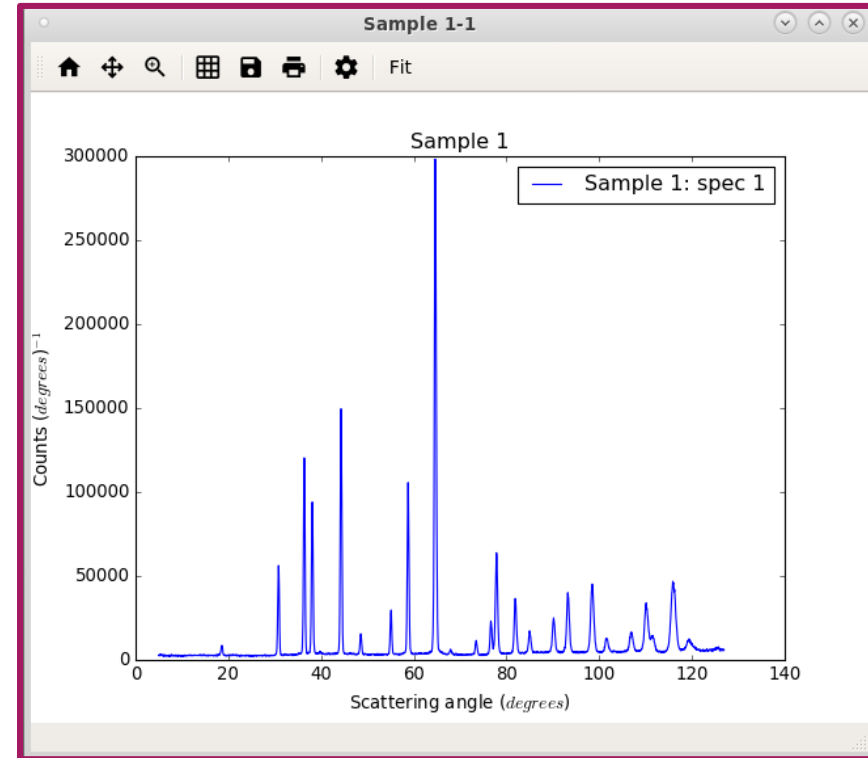


After clicking run your workspace will appear here

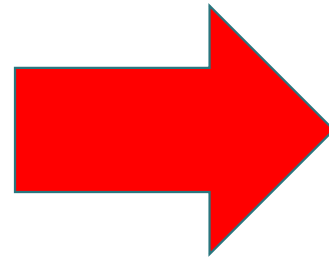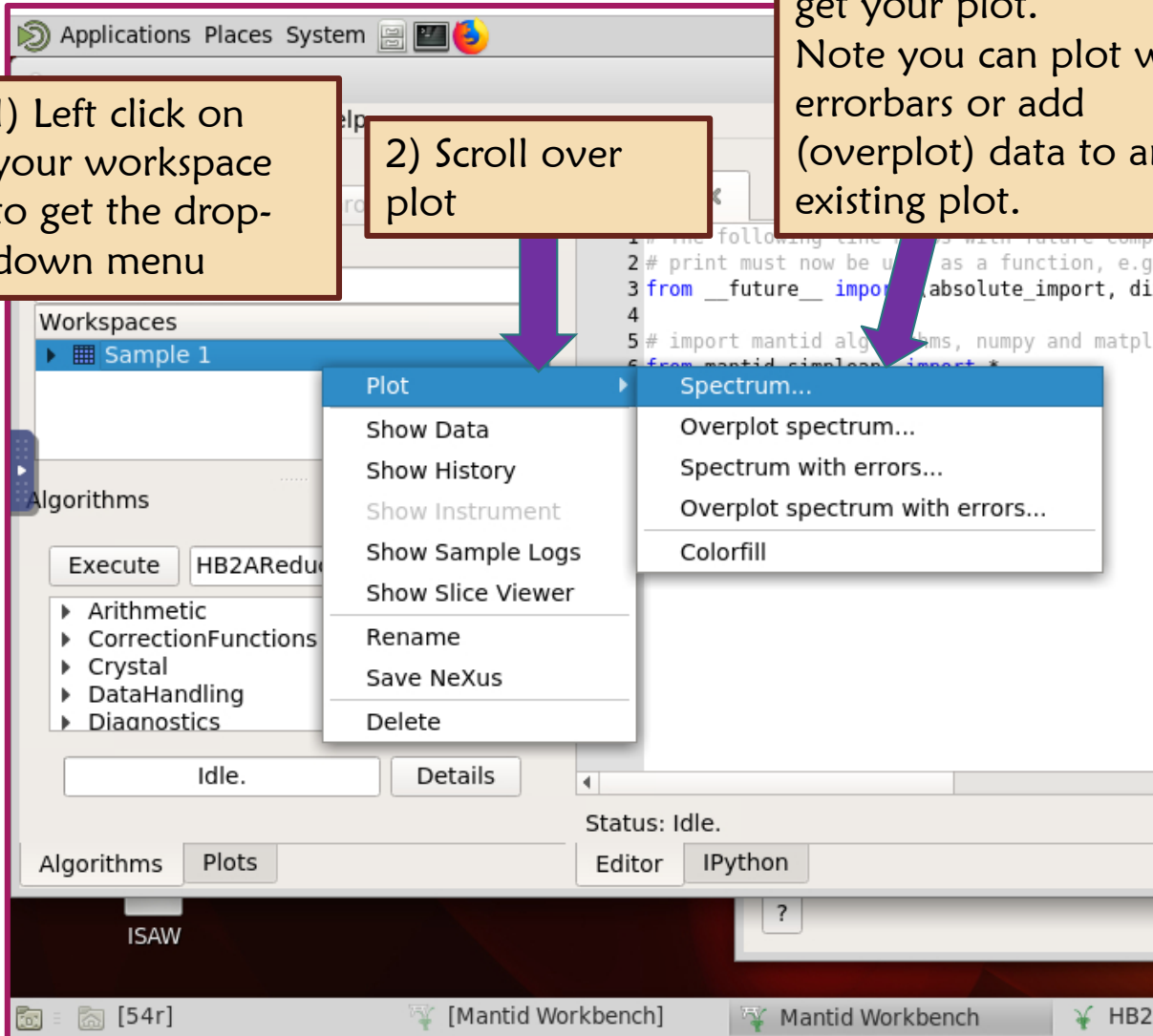# Plotting data from workspaces
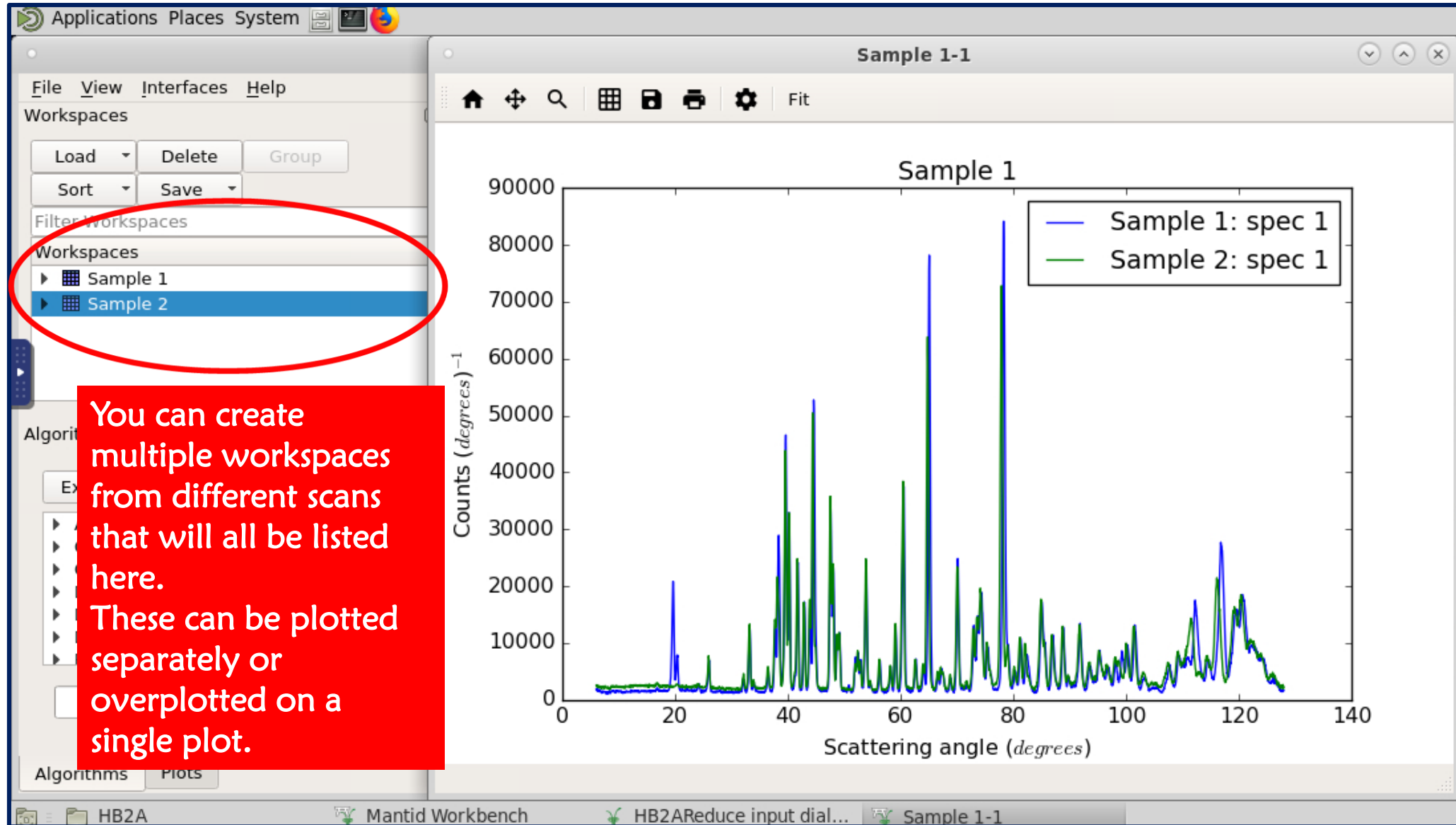
1) Left click on your workspace to get the drop-down menu

2) Scroll over plot

3) Click on Spectrum to get your plot.
Note you can plot with errorbars or add (overplot) data to an existing plot.

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# Overlaid plots



You can create multiple workspaces from different scans that will all be listed here.
These can be plotted separately or overplotted on a single plot.

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# Plotting individual detectors

- Order parameter measurements on HB2A are run to follow the intensity of a single detector as the temperature (or field/pressure) is controlled.

- These can be plot using the same HB2AReduce dialogue window.

- The procedure is described in the following steps

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# Plotting a single detector

2) Follow the same steps you would as if you were plotting a standard diffraction pattern

3) This box should appear. Put the individual detector that you want *(This will be known to you and the instrument team when running the scan and idshould be included in the scan title when the scan is run)*
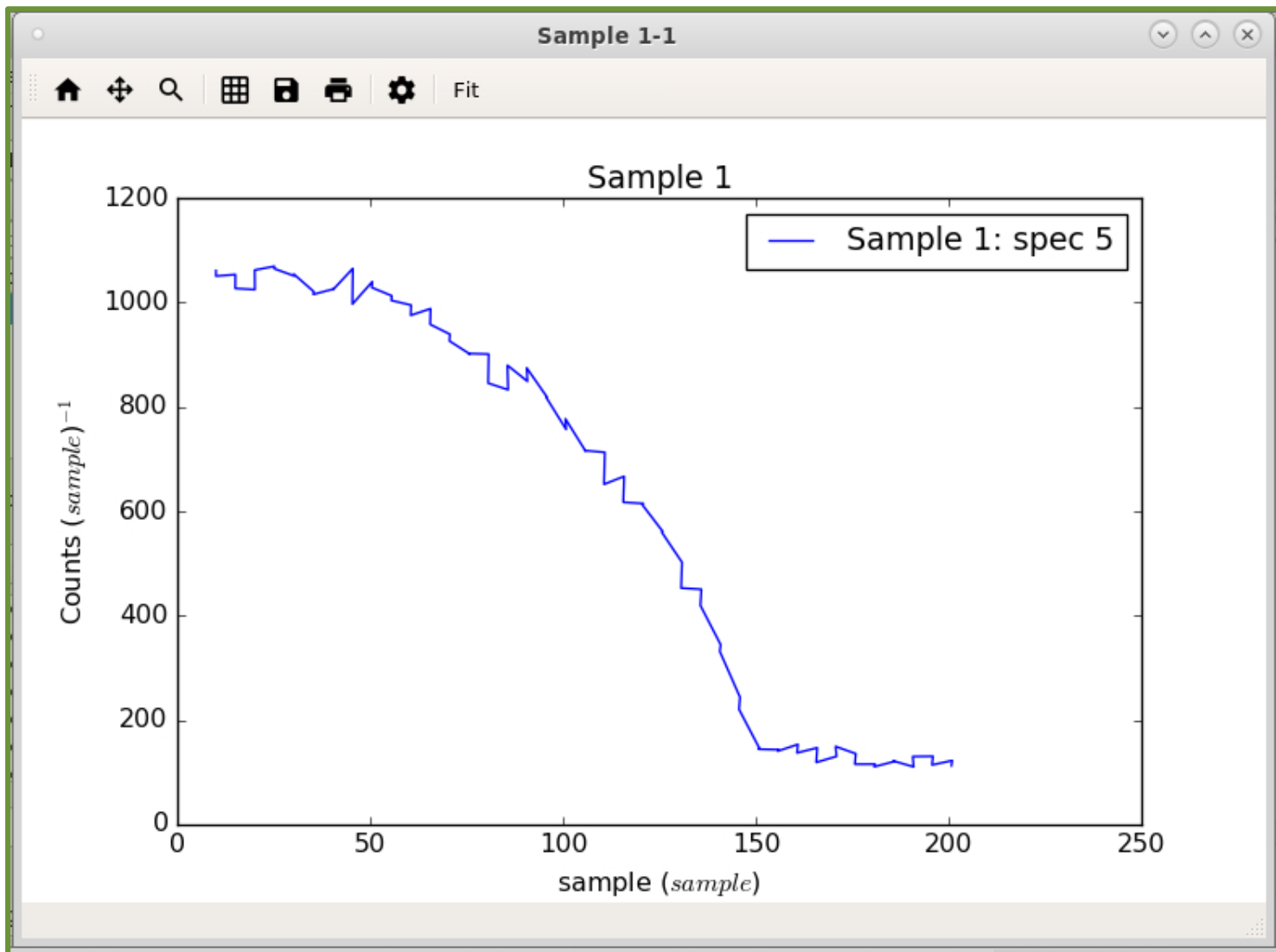
4) The detector you selected should appear.
Detector 5 in this case.

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# How to manually save your data

**3) This box should appear**

This is the workspace you want to save. If you have executed more than one workspace, there is a drop-down function to pick the workspace you want to use

This is where you name your data

This is the format you would like to save it in
*The next slide will show all the formats the file can be saved as

If you want to keep this box open, click this

When you are ready to run the algorithm click here

## SaveFocusedXYE input dialog

Saves a focused data set (usually the output of a diffraction focusing routine but not exclusively) into a three column format containing $X_i$, $Y_i$, and $E_i$.

| InputWorkspace | Sample 1 ▼ |
| **Filename** | Run 1 | Browse |

☑ SplitFiles

| StartAtBankNumber | 0 |

☐ Append

☑ IncludeHeader

| Format | XYE ▼ |

Keep Open ☑ | Run | Close

?

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**SaveFocusedXYE input dialog**

Saves a focused data set (usually the output of a diffraction focusing routine but not exclusively) into a three column format containing X_i, Y_i, and E_i.
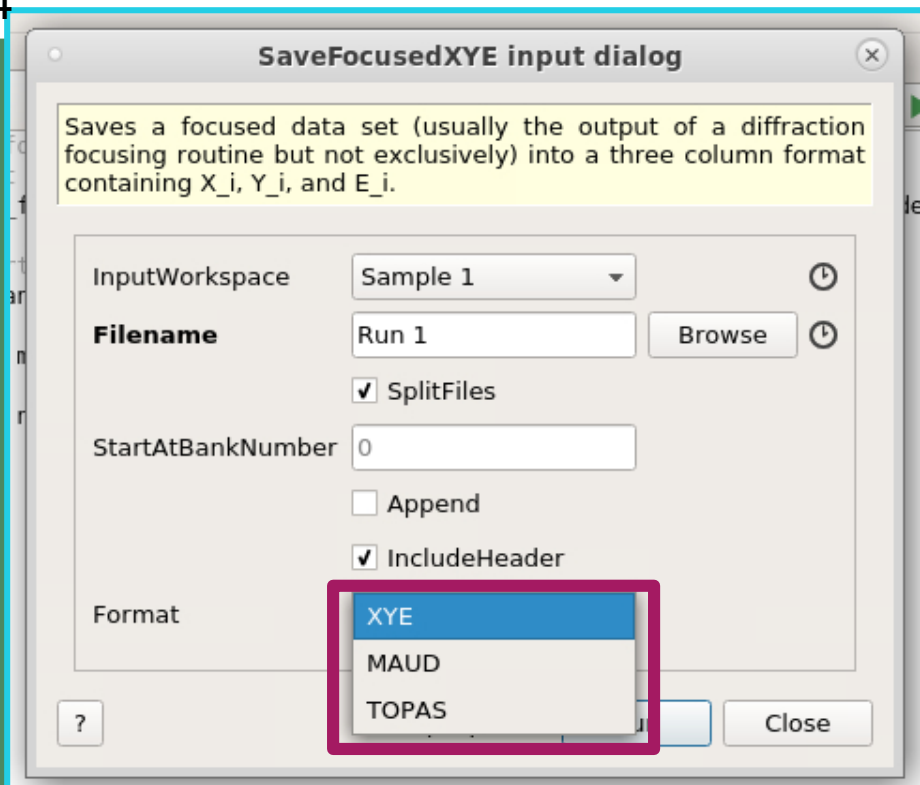
InputWorkspace: Sample 1

**Filename** Run 1 Browse
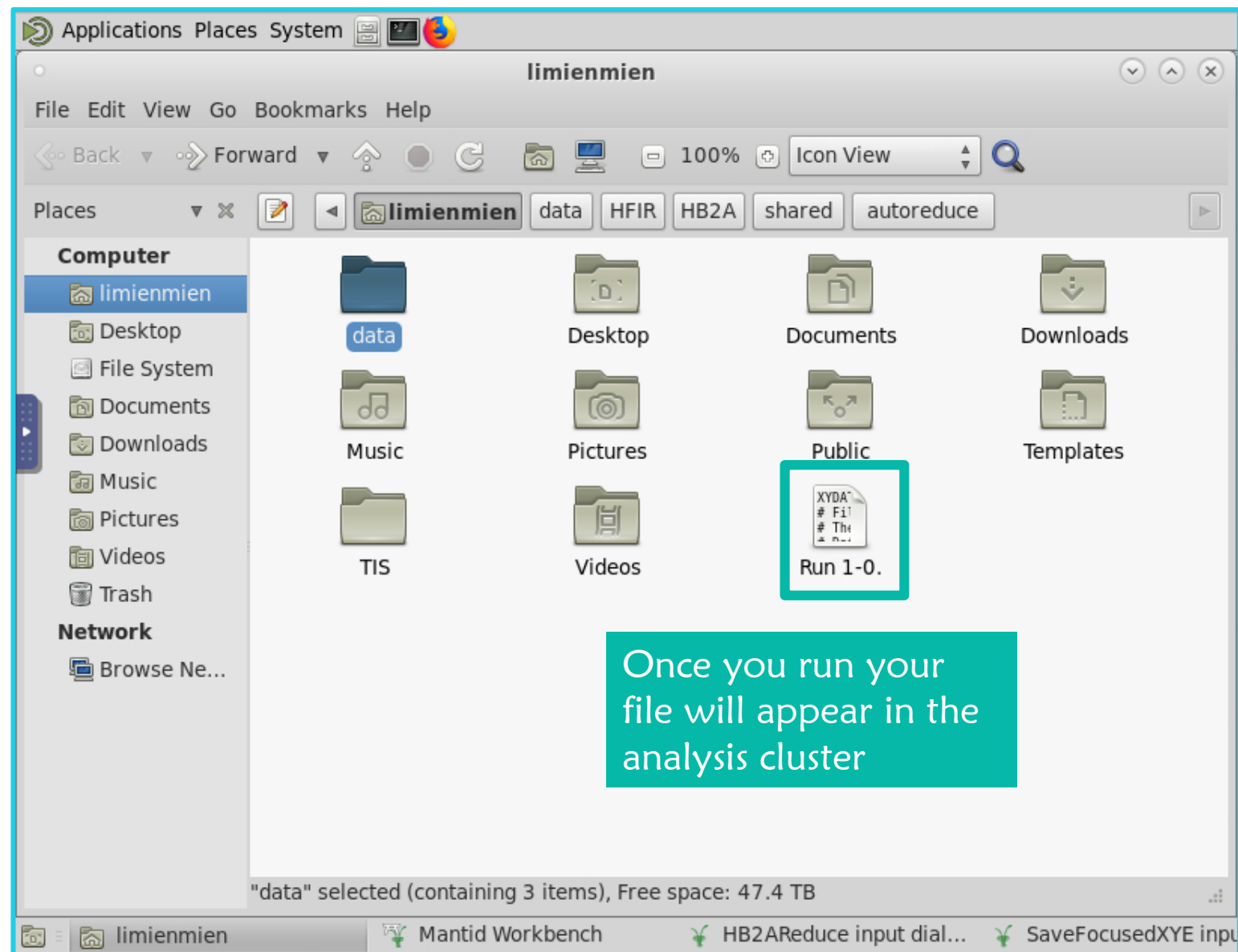
✓ SplitFiles

StartAtBankNumber 0

☐ Append

✓ IncludeHeader

Format:
- XYE
- MAUD
- TOPAS

Close

This is a drop-down menu, and you can select the format you want to save your file in

Applications Places System

**limienmien**

File Edit View Go Bookmarks Help

Back ▾ Forward ▾ 100% Icon View

Places ▾ ✕ ◀ 🏠limienmien data HFIR HB2A shared autoreduce

**Computer**
- 🏠 limienmien
- 🖥 Desktop
- File System
- 📄 Documents
- 📥 Downloads
- 🎵 Music
- 🖼 Pictures
- 📹 Videos
- 🗑 Trash

**Network**
- 🖧 Browse Ne...

data | Desktop | Documents | Downloads

Music | Pictures | Public | Templates

TIS | Videos | Run 1-0.

Once you run your file will appear in the analysis cluster

"data" selected (containing 3 items), Free space: 47.4 TB

limienmien | Mantid Workbench | HB2AReduce input dial... | SaveFocusedXYE inp

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