

ADDIE User Manual

ADvanced DIffraction Environment

Data reduction software for NOMAD

April 5, 2017 version

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Chapter 1

Introduction

1.1 What is ADDIE

The ADvanced DIffraction Environment (ADDIE) is User software for reducing and analyzing data on the **Nanoscale Ordered MAterials Diffractometer** (NOMAD) instrument at the **Spallation Neutron Source** (SNS). Now, with a full plate of acronyms, let's begin.

ADDIE provides a graphical user interface (GUI) to interact with the underlying data reduction software. ADDIE aims to guide the workflow to go from launching the reduction of raw neutron data to provided processed individual runs, post-processing of these individual runs by applying optional corrections and summations, finally to visualization and output of the diffraction and pair distribution function data.

ADDIE is pre-installed on the **Analysis** machine at the SNS (<http://analysis.sns.gov>). Instructions are provided for Neutron Sciences users to setup the Remote Desktop capabilities to view, analyze and download your data from anywhere you go. Options are provided Windows, Mac, and Linux. Also, contact support information is provided in the case of any issues or needed troubleshooting.

ADDIE is also available open-source. Please contact your Local Contact from NOMAD if you would like to know more about the repository (or to contribute!)

1.2 Using ADDIE

ADDIE development has been funded by the [US Department of Energy](#) (DOE).

If you use ADDIE results in your published work, please cite the following papers:

(INSERT - ADDIE paper) (INSERT - other reduction dependencies - Mantid, GUDRUN, etc.)

For any of the following features for your published work, please cite the associated papers:

(INSERT - specific feature papers)

From the following, you can download a [BibTex file with all citations](#).

Chapter 2

Getting Started

2.1 Background

What does ADDIE actually do during data reduction? For each run, we must have the following measurements for data reduction:

$$\begin{aligned} I_{sample} &= \text{sample intensity} \\ I_C &= \text{sample container intensity} \\ I_{Cb} &= \text{container background intensity} \\ I_V &= \text{vanadium intensity} \\ I_{Vb} &= \text{vanadium background intensity} \end{aligned} \tag{2.1}$$

Why all these measurements for a single run? We want to measure only the coherent sample scattering (I_{sample}^{coh}). Unfortunately, we cannot suspend the sample in space inside the instrument. We must have a sample container. Thus, we measure the empty sample container intensity (I_C) in the instrument to subtract this from the sample scattering intensity (I_{sample}). Yet, we can have many different types of "containers" (i.e. sample environments such as a furnace or

cryostat, vanadium cans, quartz tubes, tubes in cans, etc.) Therefore, we must correct "from the outside in" where we subtract a completely empty instrument from the outermost containment scattering intensity, then subtract this from the next layer of containment and continue till we reach the sample subtracted (I_{sample}) from this collective background ($I_C + I_{Cb}$). Also, we do not know the exact beam profile to put the sample scattering intensity on an absolute scale. For this, we use vanadium to normalize the sample scattering intensity to extract the coherent scattering (I_{sample}^{coh}) from the incoherent scattering (I_{sample}^{inc}) on an absolute scale.

Why vanadium for normalization? We use vanadium for a few different reasons. 1) Vanadium has a small coherent scattering length but is a great incoherent scattering material. Thus, it does not contain large Bragg reflections in its profile that would have to be removed but provides a well-defined total beam profile. 2) Vanadium is a solid metal with well known density and stable without a container. 3) The large mass of vanadium atoms reduces the need to correct for inelastic scattering effects.

What else before we get our coherent sample intensity? Last, we must take into account the loss of intensity of the neutron beam as it passes through every material present in the experiment. To some degree, the sample, container, and vanadium will all attenuate the neutron beam. Ignoring the sample attenuation, we have:

$$I_{sample}^{coh} = \frac{I_{sample} - \alpha_c(I_C - I_{Cb})}{\alpha_v(I_V - I_{Vb})} \quad (2.2)$$

From the coherent scattering, we have the total scattering structure function given as:

$$\begin{aligned} S(Q) - 1 &= \frac{\frac{I_{sample}^{coh}}{N} - \langle b^2 \rangle}{\langle b \rangle^2} \\ &= \frac{\frac{d\sigma}{d\Omega} - \langle b^2 \rangle}{\langle b \rangle^2} \\ &= \end{aligned} \quad (2.3)$$

where $\langle b \rangle^2$ and $\langle b^2 \rangle$ are the squared average and average squared scattering power of the sample where:

$$\langle b \rangle = \frac{\sum_i^N b_i}{N} \quad (2.4)$$

where b_i is the scattering power of atom i and N is the total number of atoms in the sample.

The pair distribution function (PDF) is obtained from the Fourier transform of $S(Q) - 1$:

$$G(r) = \frac{2}{\pi} \int_{\text{inf}}^0 Q[S(Q) - 1] \sin(Qr) dQ \quad (2.5)$$

2.2 Specifics of NOMAD data reduction

To obtain $S(Q)$ we using the following:

$$S(Q) - 1 = \frac{\frac{I_{sample}^{coh}}{N} - I_{poly}}{I_{poly}} \quad (2.6)$$

where

$$I_{poly} = \begin{cases} \frac{\rho\sigma d^2}{\rho_v \sigma_v d_v^2} & hyd = -1 \\ a_0 + a_1q + \dots a_n q^n & hyd = 0 \\ xL(q_0) + (1-x)G(q_0) & hyd = 2 \end{cases}$$

absolute normalization
 requires knowledge of sample properties
 not done in autoreduction
 least-square polynomial fit
 of q-region qminpla < Q < qmaxpla
 non-linear least square fit to pseudo-Voigt function.
 $L(q)$ = Lorentzian, $G(q)$ = Gaussian
 Used for samples containing hydrogen or deuterium

Chapter 3

Workflow for Data Reduction

To launch ADDIE, you must:

1. Login to the **Analysis** machine
2. Open a terminal
3. Navigate to your IPTS. It will be located on Analysis under `/SNS/NOM/IPTS-<your experiment ID>`
4. Launch ADDIE using the command: `fastgr`
5. Wait for the GUI to appear

3.1 Launch automatic data reduction of individual runs

3.1.1 Raw neutron event files

Once the samples are in the beam, the experiment is setup, and you begin collecting data in runs, raw neutron events will begin being saved in files. Raw neutron events are every instance of a neutron being detected by a detector.

For NOMAD at the SNS on the [Analysis](#) machine, the saved files are NeXus files located in your IPTS folder under `/SNS/NOM/IPTS-<your experiment ID>/nexus`. These are permanent files that cannot be edited or deleted. In these files are the neutron event data and also the metadata associated with the run (i.e. what temperature a probe is reading, what are the chopper settings, sample information).

These raw neutron event files are what we reduce to get to the useful data for our material. This process is referred to as data reduction.

Examining NeXus files

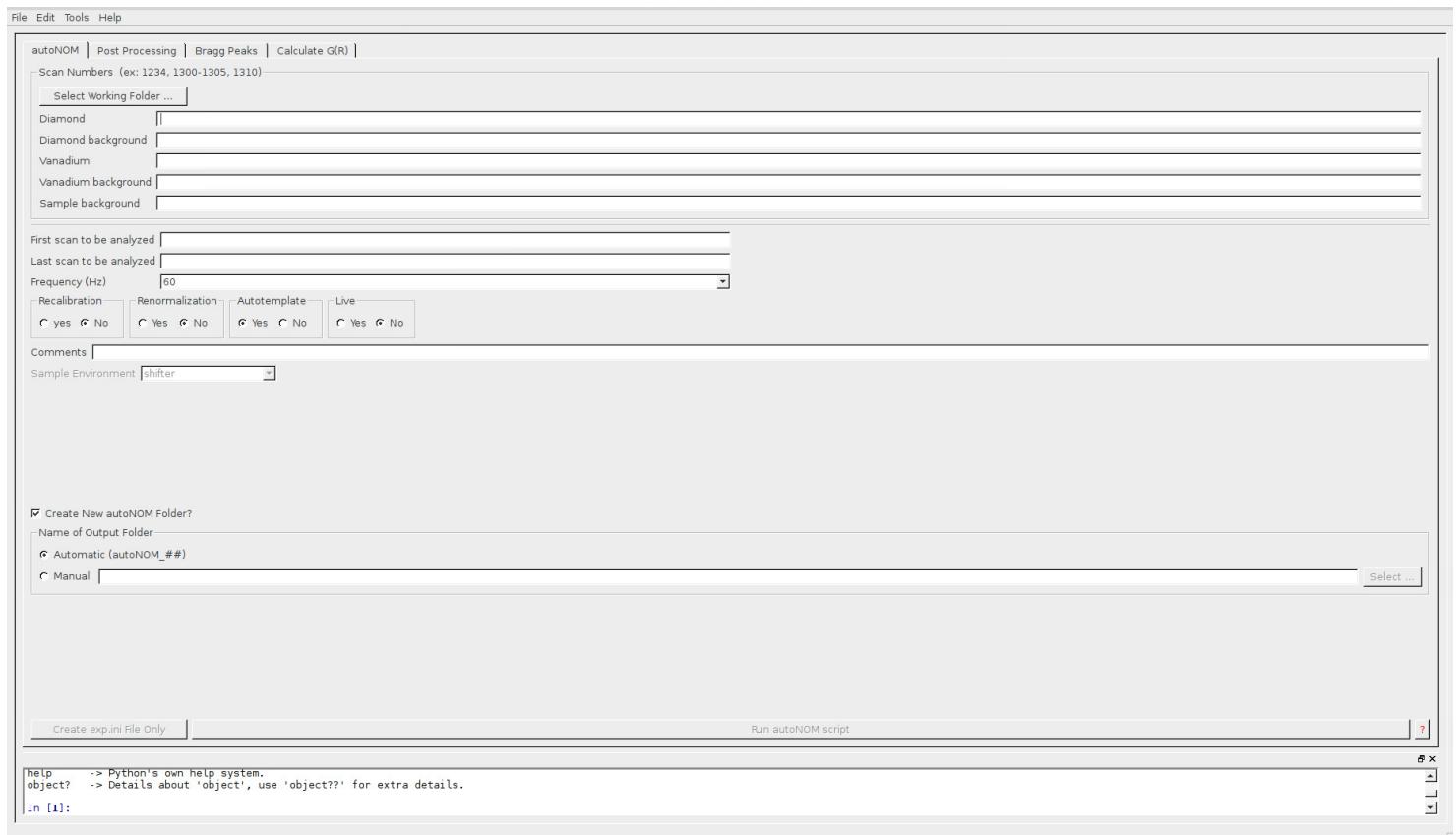
You can examine the NeXus files from the command line of a terminal using `nxbrowse <NeXus filename>`. These files have a directory structure. You can `ls` to list the current level of the directory and use `cd` to enter a directory. All these files have the `entry` as the initial entry point. Then, if you `ls`, you will see that there are entries with the attributes `NX Group` and `NX Data`. For any entry with the attribute `NX Data`, you can use `read <entry>` to read the value of this entry. For any with the attribute `NX Group`, this is a sub-level directory associated with this entry. You can `cd` into the `NX Group` and then proceed with using `read`. To exit the NeXus file, you can use `exit` at any time to return to the terminal.

3.1.2 Experiment Information Input

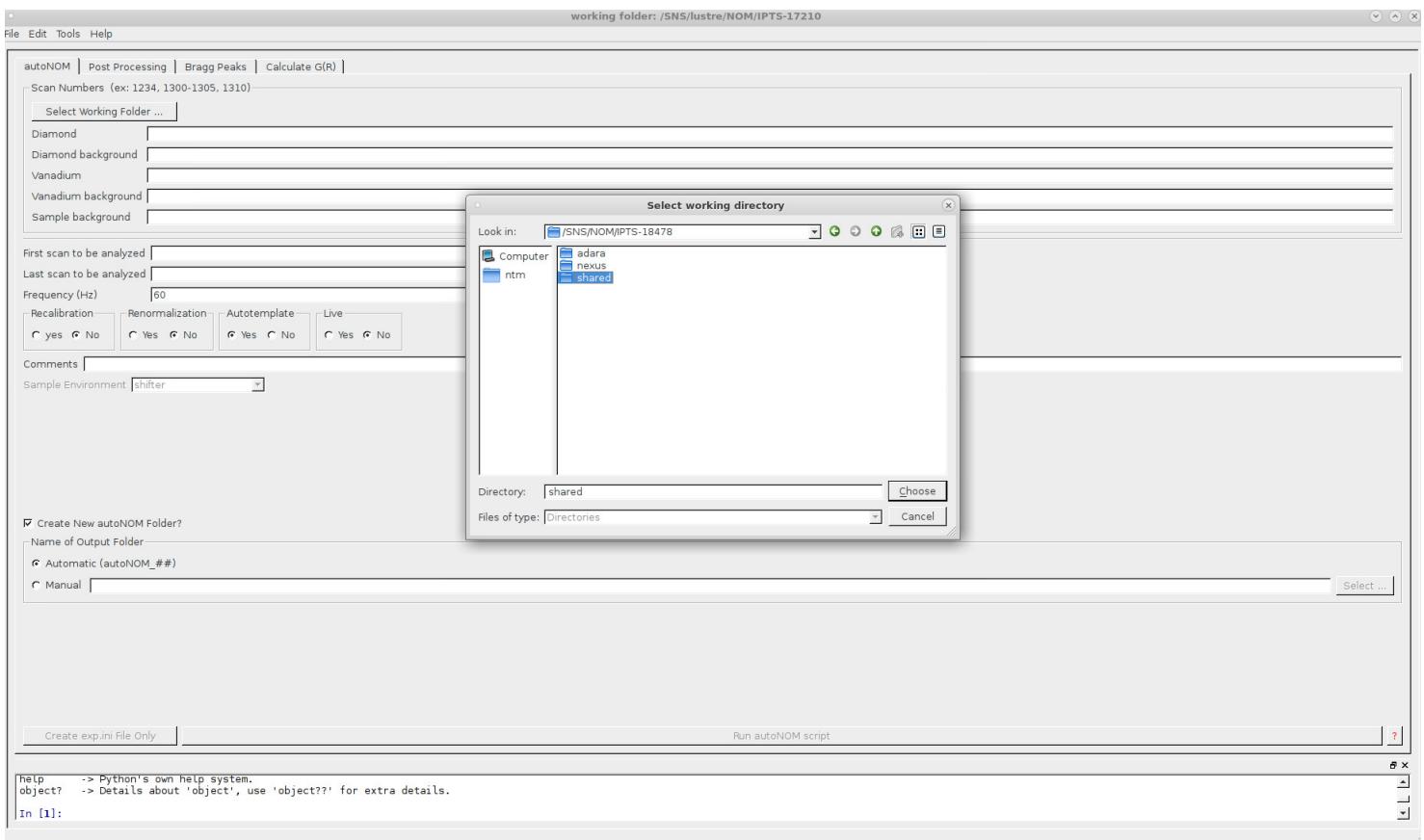
ADDIE can be used to launch an automated data reduction, or autoreduction, of your sample runs as they complete and produce NeXus files. The autoreduction processes the NeXus files as they appear under your IPTS folder.

Loading In the Experiment Information

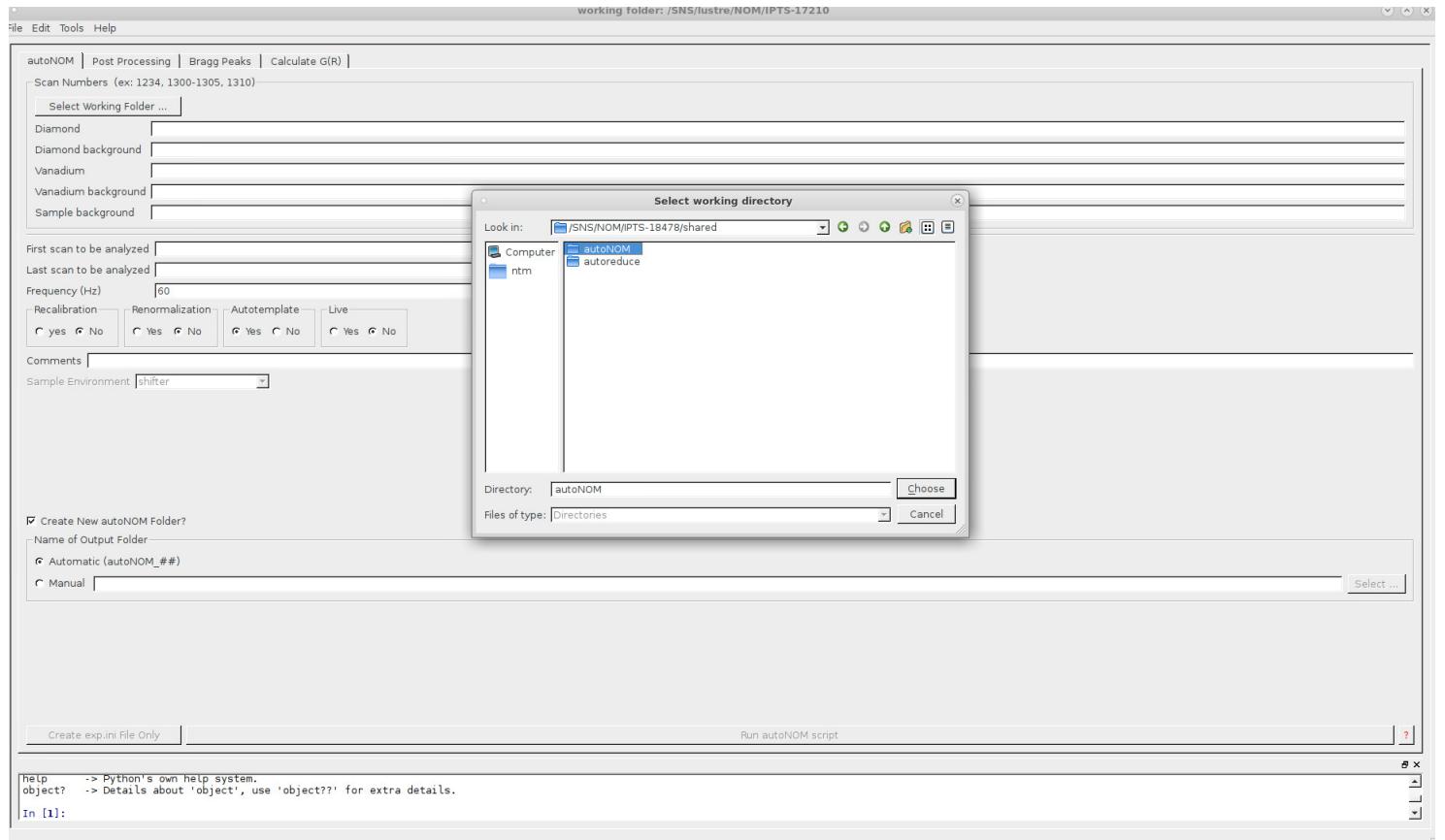
To setup the autoreduction, first launch ADDIE as described before. You will begin with the following screen with the autoreduction tab open:



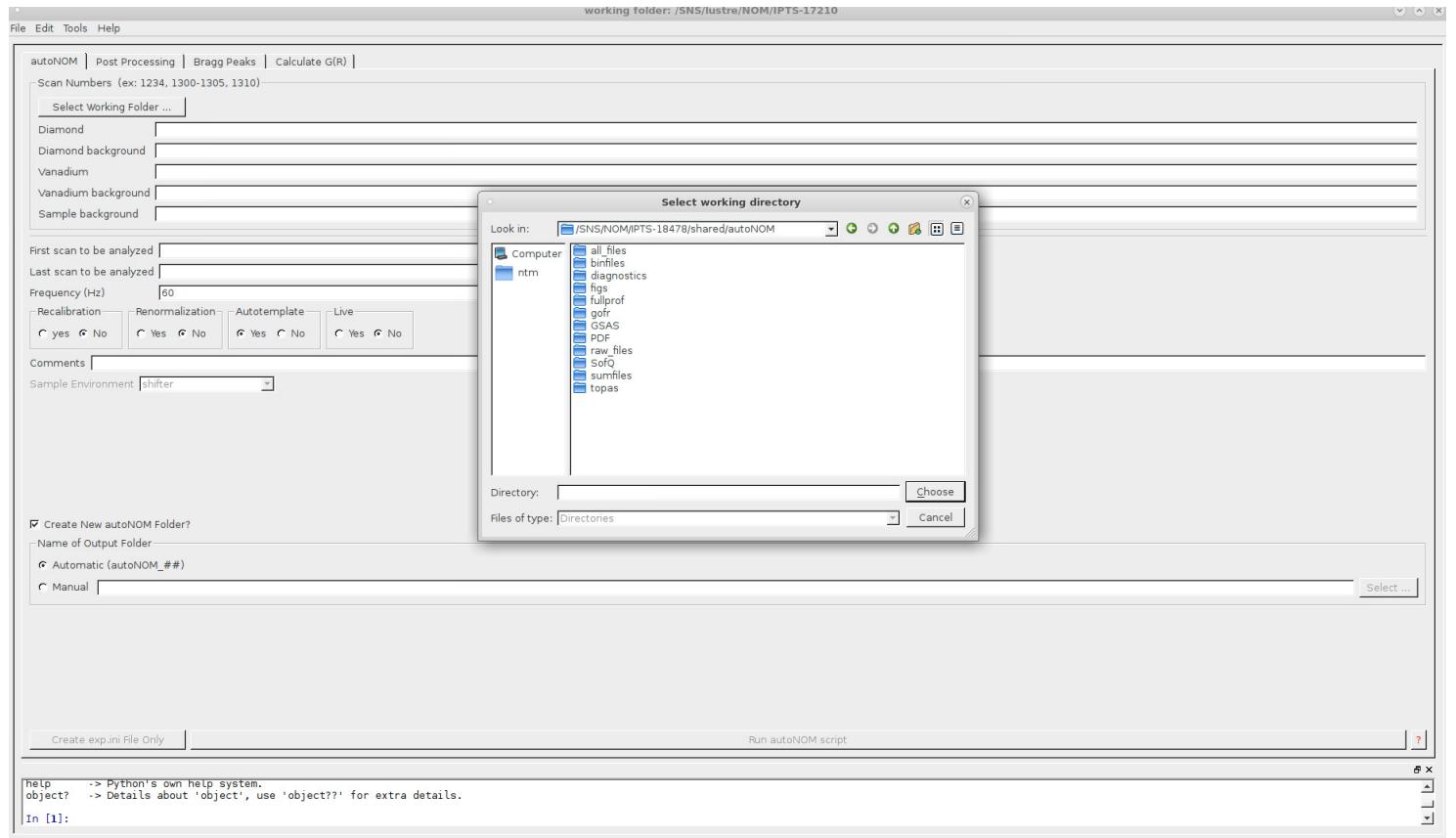
Here, we input the run numbers for the necessary measurements specified in Equation 2.1 in order to create our reduced data, Equation 2.2. To read in this data from an experiment input file (the `exp.ini` file), click on the **Select Working Folder...** button at the top. You will be presented with a dialog box that will prompt you to select a working directory. It will begin with your current working directory, which you can see displayed at the top in the **Look in:** field. If you are in your `/SNS/NOM/IPTS-<your experiment ID>` directory, you should get something as below:



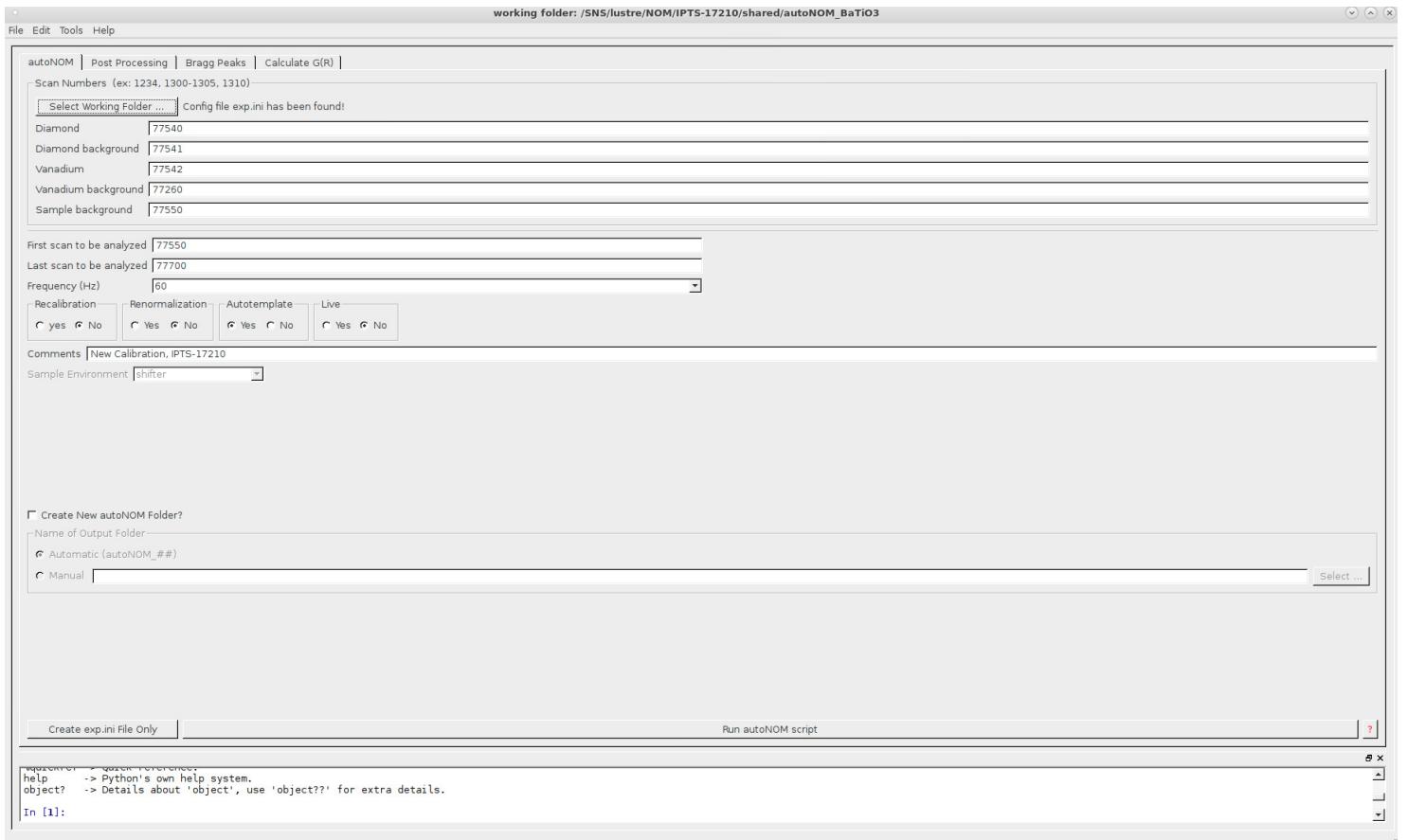
This is the file directory structure of your IPTS. You can see the `nexus` directory where the raw neutron event files are stored, the `adara` directory (ADARA = Accelerating Data Acquisition, Reduction, and Analysis) for automated live reduction files, and the `shared` directory, which is a User workspace for the experiment. Double-click the `shared` directory and you will see something similar to the following:



Here, the **autoNOM** directory is where we will kick off the autoreduction of AD-DIE. This will produce the **autoreduce** directory that you see above. This IPTS has already had the data reduction performed. If your IPTS has not yet had the data reduced, you may not see either of these directories. If the **autoNOM** directory does not exists, go to the terminal, get to the shared directory above (`cd /SNS/NOM/IPTS-<your experiment ID>/shared`) and create it using the command: `mkdir autoNOM`. Once this directory exists, double-click the **autoNOM** directory. You will see something similar to the following:



Again, we have already launched data reduction in this IPTS so you see the directories that will be produced. For now, simply select **Choose** on the bottom left. This will look for the experiment input file (the `exp.ini` file) in the current directory. If the file is found, the tab should populate with the experiment information in the file and look similar to the following:



If no experiment file was found, you will see the following next to the **Select Working Folder...** button:



If this occurs, you can fill in the necessary fields. Once you have these filled in, you can output an experiment input file using the **Create exp.ini File Only** button. Yet, this file will be automatically created once we kick off the autoreduction.

The experiment input file (`exp.ini` file) has the following format:

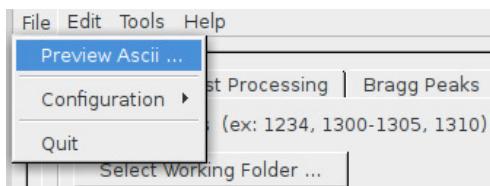
```
required ****
Dia 77540
DiaBg 77541
Vana 77542
VanaBg 77260
MTc 77550
optional ****
recali no
renorm no
autotemp yes
scanl 77550
scanol 77700
Hz 60
# New Calibration, IPTS-17210
```

If No Experiment Information File Exists

If you do not know these run numbers required to begin processing your data but you have measured them in your current IPTS, you can create a List of Scans file (a `los.txt` file) that has this information using the following command on the command line of a terminal:

```
python /SNS/NOM/shared/autoNOM/stable/readtitles.py
```

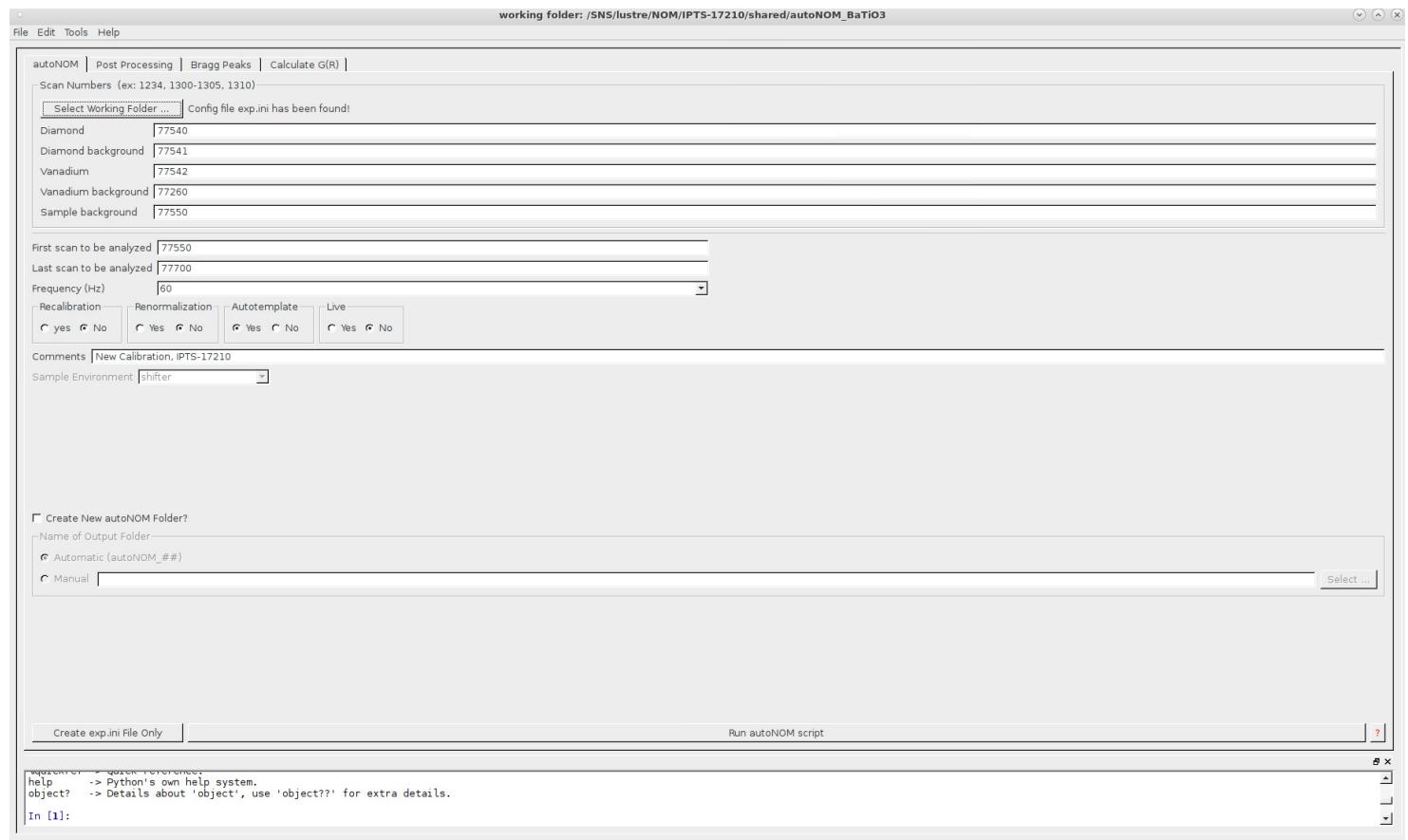
You can open this file (`los.txt` from ADDIE by going to the *File* drop-down from the *Menu* bar and selecting the *Preview Ascii...* and selecting the `los.txt` file. You can optionally use a text editor (`gedit`, `vim`, `emacs`) from a terminal.



If you have any trouble with this step, please contact your Local Instrument Scientist Contact to help you get the necessary files. These can even be located in a directory you do not have access to, in which case, the Instrument Scientist can help assist you and ensure you have all the necessary files to launch the data reduction.

3.1.3 Setting up Data Reduction

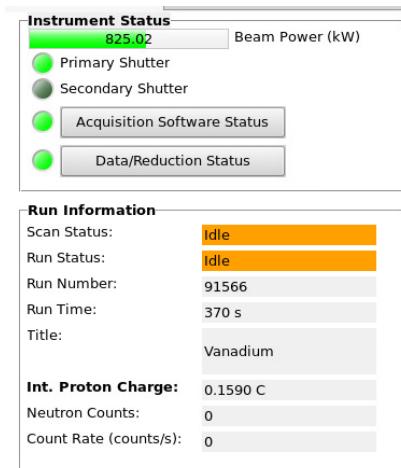
At this point, you should have experiment information input into the tab similar to the following:



If you have questions about the run numbers (Diamond, Vanadium, Backgrounds, etc.) and what they are used for, please refer to Section 2.1 for an explanation.

Settings:

- ***First scan to be analyzed:*** we input the first run number of your IPTS. This can be found from the DAS where you setup the experiment and are controlling the instrument. It will be under **Run Information** as **Run Number**, similar to the following where the run number is 91566:



- ***Last scan to be analyzed:*** The last run to be analyzed. If you are running a "live" experiment, you can set this to an arbitrarily large run number. Only run numbers with associated NeXus files under the current IPTS will be found and reduced.
- ***Frequency:*** Change the frequency mode of the data reduction. You can select from either 60 Hz (use every proton pulse that hits the target) or 30 Hz (use every other proton pulse). You can use the 30 Hz mode to use longer times-of-flight and thus longer wavelengths. Typically, we operate in the 60 Hz mode.
- ***Recalibration:*** Either use the current calibration files present or re-

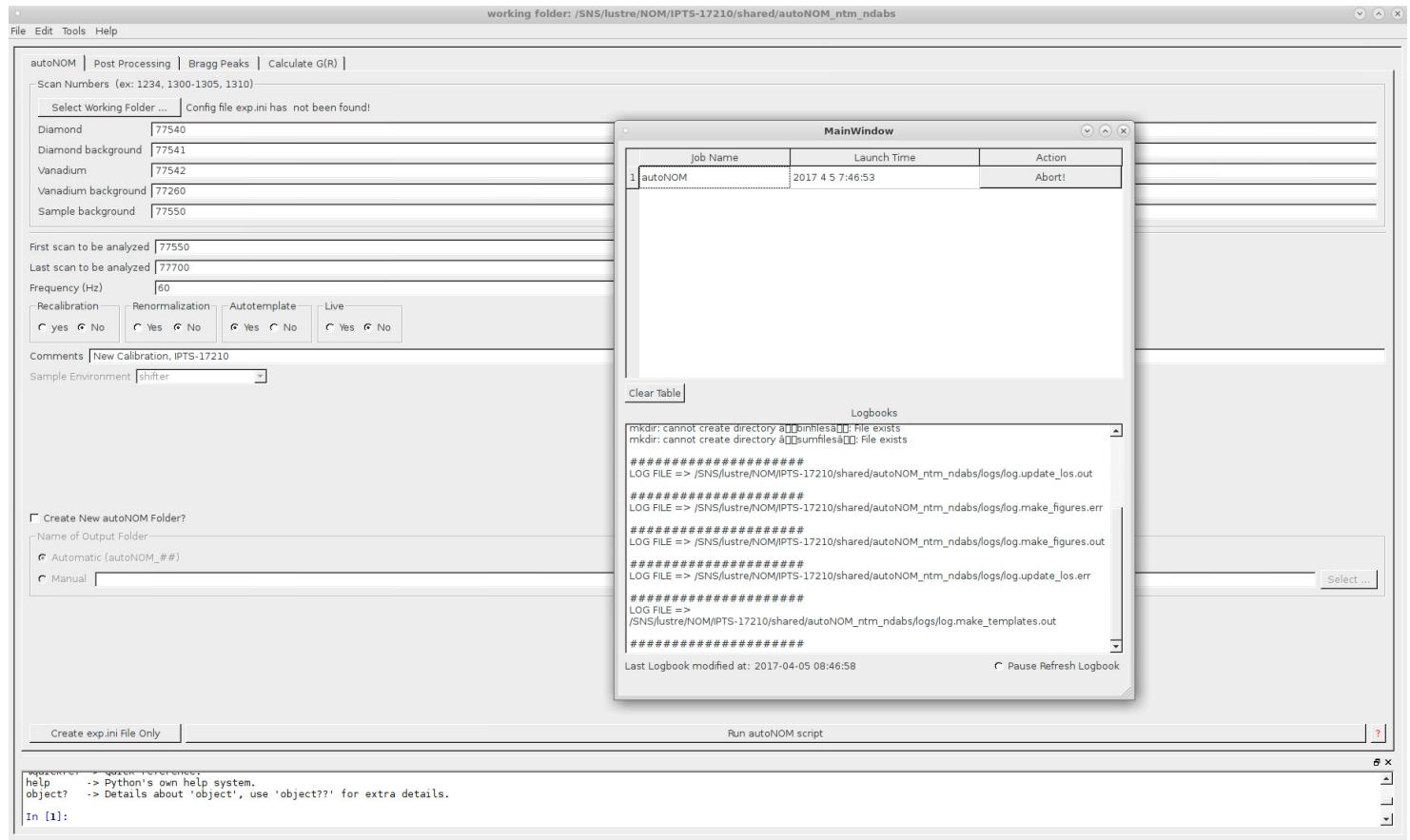
perform calibration using the input Diamond run. If the re-calibration is set to No but no calibration files are found, it will automatically perform the calibration again.

- ***Renormalization***: Either use the current normalization files present or re-perform calibration using the input Vanadium run. If the re-normalization is set to No but no normalization files are found, it will automatically perform the normalization again.
- ***Autotemplate***: Setup an organized directory structure under the autoNOM parent directory. Always recommended and preferred.
- ***Live***: Launch data reduction in either live mode where NeXus files will continuously be produced or in a post-processing mode where data reduction will stop once the last scan is analyzed.
- ***Comment***: This is a place to store a metadata comment about the experiment input information. Examples would be in what IPTS were the diamond and vanadium runs used from if they did not come from this IPTS, what was the sample environment, and any other information. This will be stored in the experiment input file (the `exp.ini` file).
- ***Sample Environment*** Specifies the sample environment. Used to determine if a calibration already exists for this sample environment.
- ***Create New autoNOM Folder?***: When data reduction is launched, this will create a new autoNOM directory and work within that folder. If you have already made an autoNOM directory, uncheck this box or you will have an autoNOM directory inside another autoNOM directory. You can let the autoNOM directory be automatically named sequentially or you can manually input the name of the directory.

3.1.4 Launch Data Reduction

Once the data reduction is setup and ready, you can kick off the automatic data reduction by pressing the ***Run autoNOM script*** button. If everything

is okay, you should see the Job Monitor window appear with the status of the job:

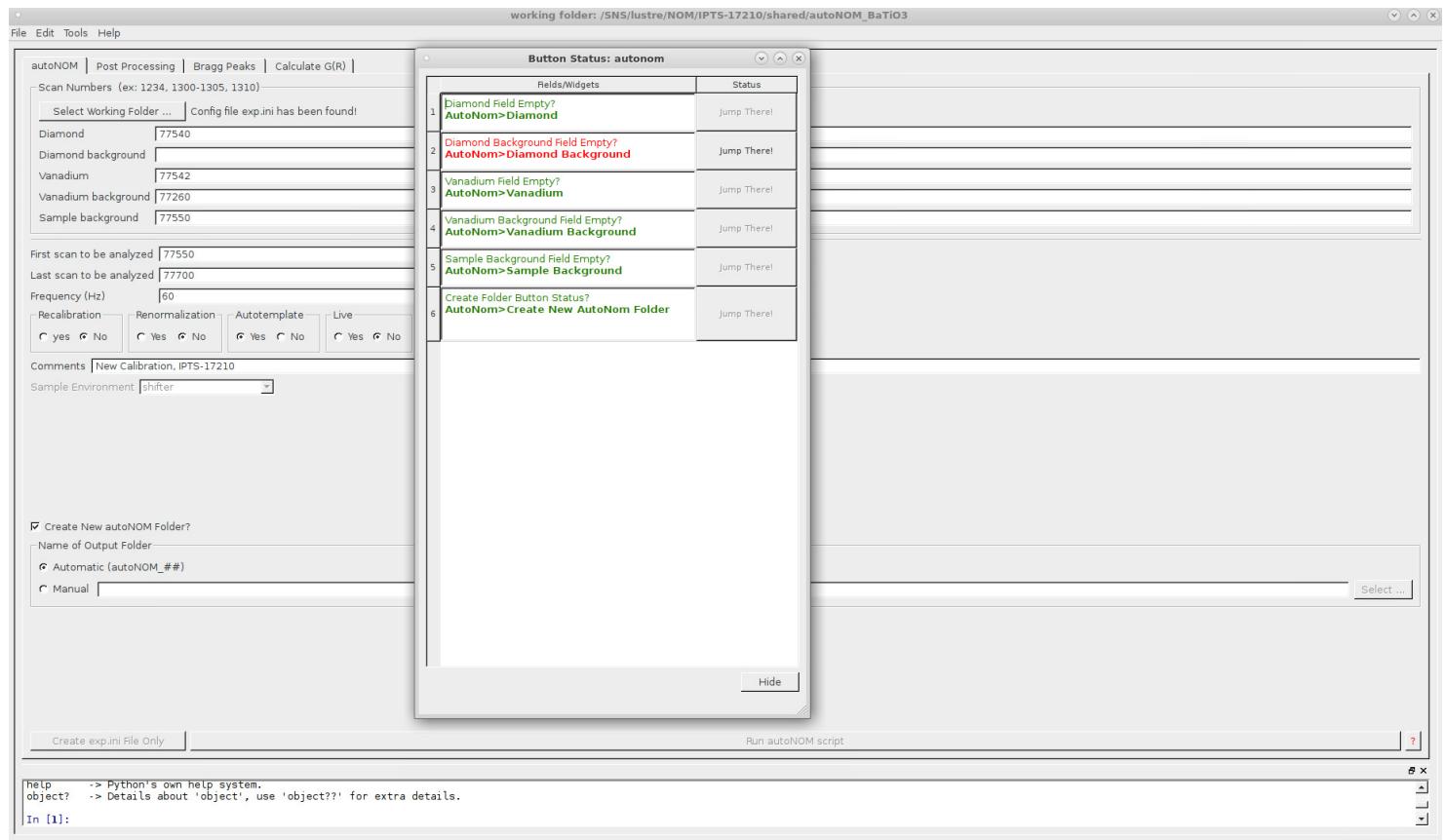


If not running in "Live" mode, you will see a display of ***Done!*** when the job is complete.

The Logbooks in the Job Monitor window display the output from log files that are saved and located in the `logs` directory under the parent autoNOM directory. Only the most recent Logbooks are displayed. The Logbook view is updated every 5 seconds by default. If you would like to pause the Logbook to scroll up and see the output, you can check the ***Pause Refresh Logbook*** radio button at the bottom. Once you are done and want to refresh the Logbook, simply press the same button again to uncheck it.

If, at any time, you need to stop the data reduction, you can press the ***Abort!*** button to kill all the running processes associated with the job. You will see a display of ***Killed!*** when the job is finished aborting.

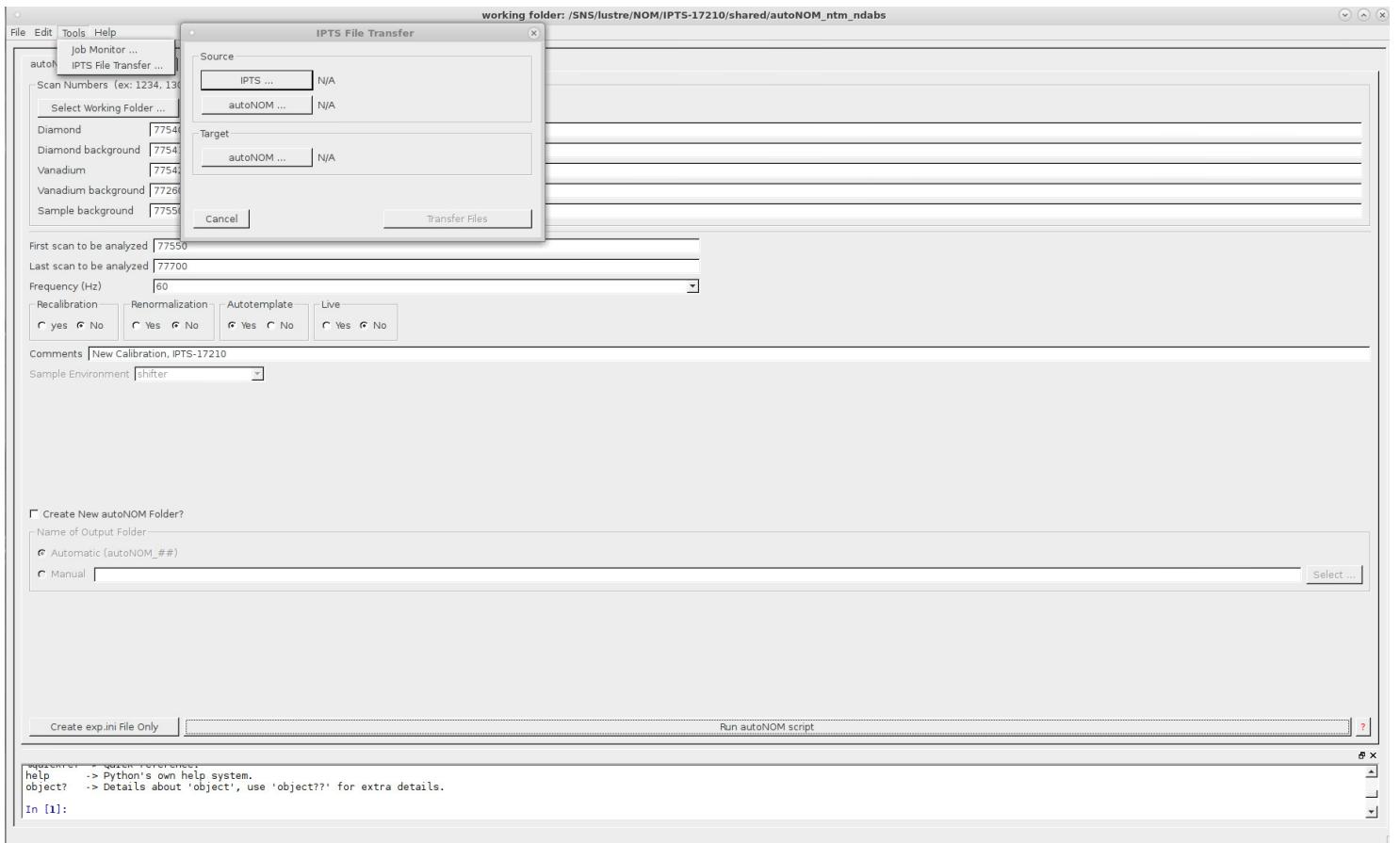
If the ***Run autoNOM script*** button is greyed out and you cannot select it, something is missing from the data reduction setup. Press the question mark button located beside the ***Run autoNOM script*** button and you will be shown what is missing in the pop-up Button Status window. Below, we have forgot the Diamond background:



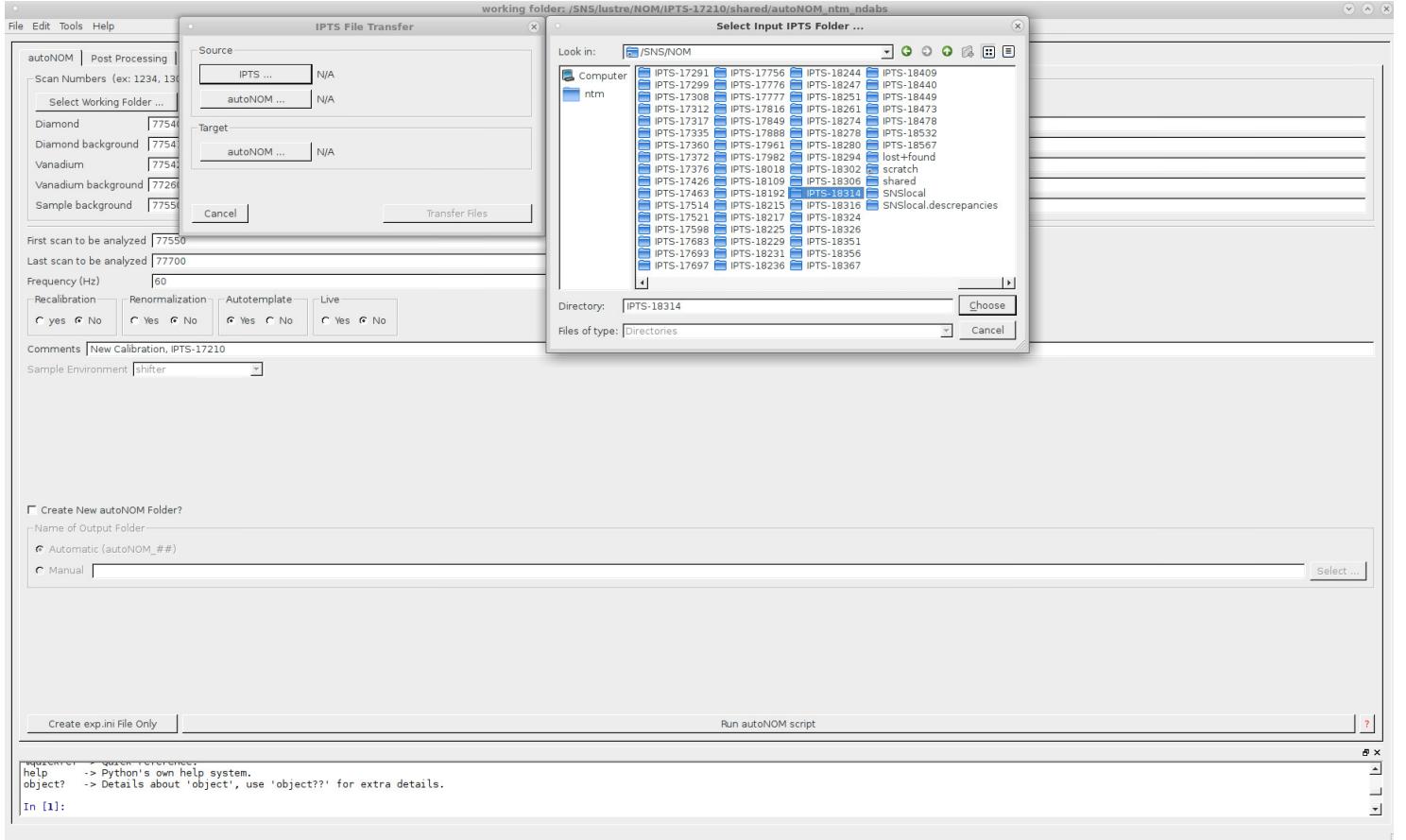
3.1.5 Getting files from another IPTS

If the diamond, vanadium, and background runs were processed in another, you can use the IPTS File Transfer tool to move over those files and bypass the need to repeat the calibration and normalization steps. **NOTE:** On the **Analysis** machine, you must have the necessary permissions to access another IPTS. This may need to be performed by an Instrument Scientist with the correct permissions. If the runs exist in another IPTS but have not been processed yet, then you can proceed as normal. If you have the necessary permissions, calibration and normalization will continue as if those files were in your IPTS.

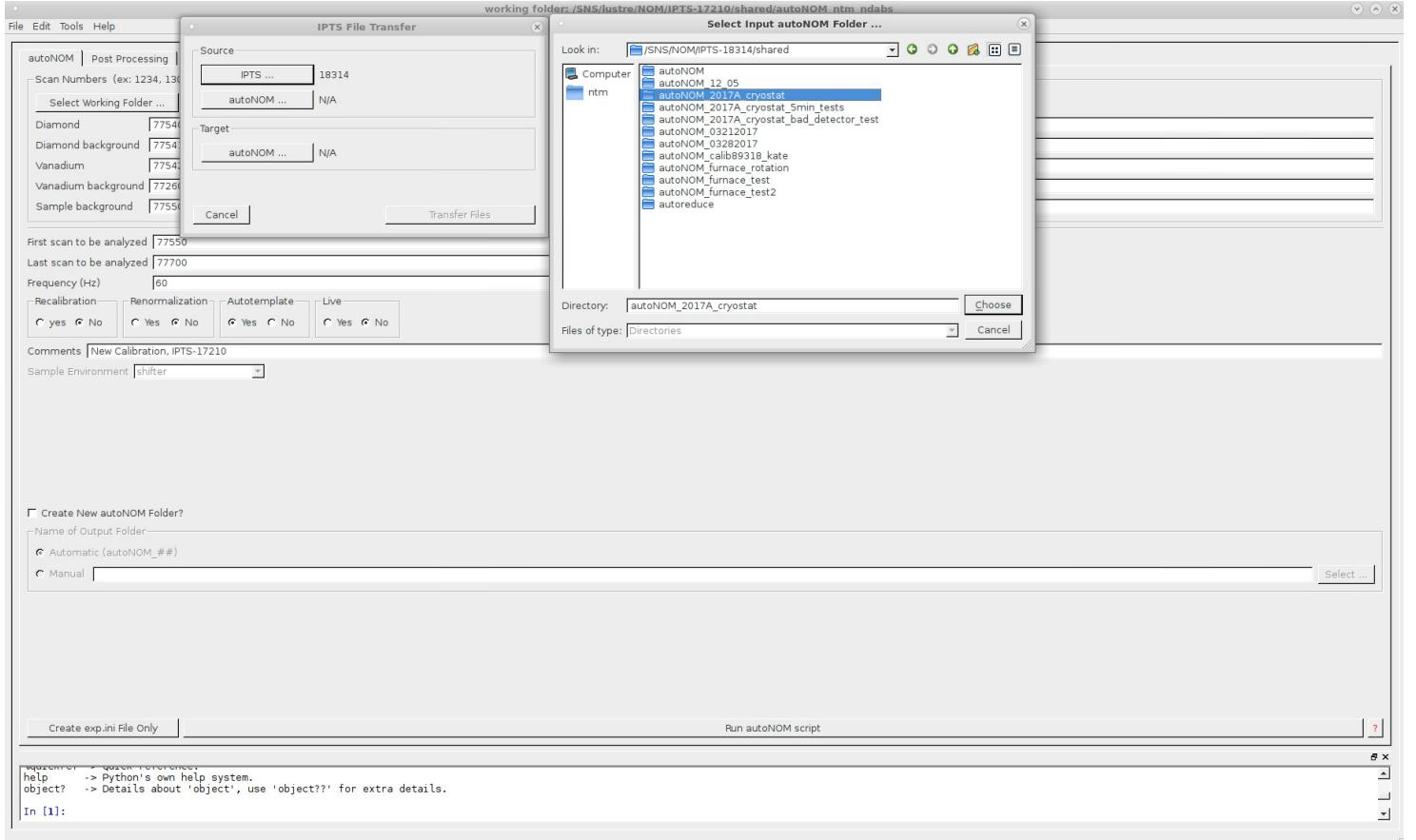
To transfer files from another IPTS, go to the **Tools** drop-down of the **Menu** bar and select **IPTS File Transfer....** You will be presented with the following dialog box:



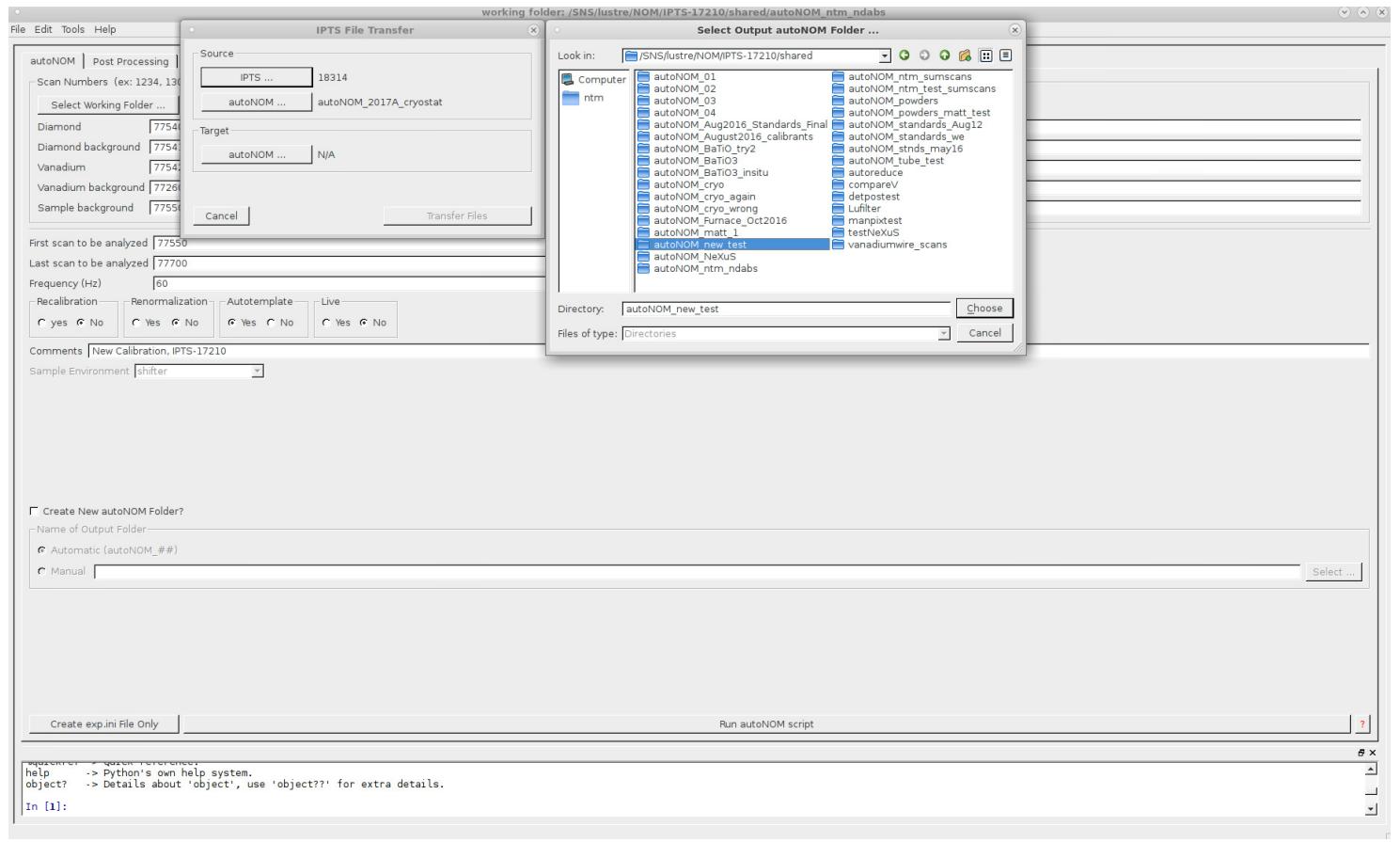
First, press the **IPTS...** button to select the IPTS from the pop-up box. Here we are selecting IPTS-18314. Press **Choose** once selected::



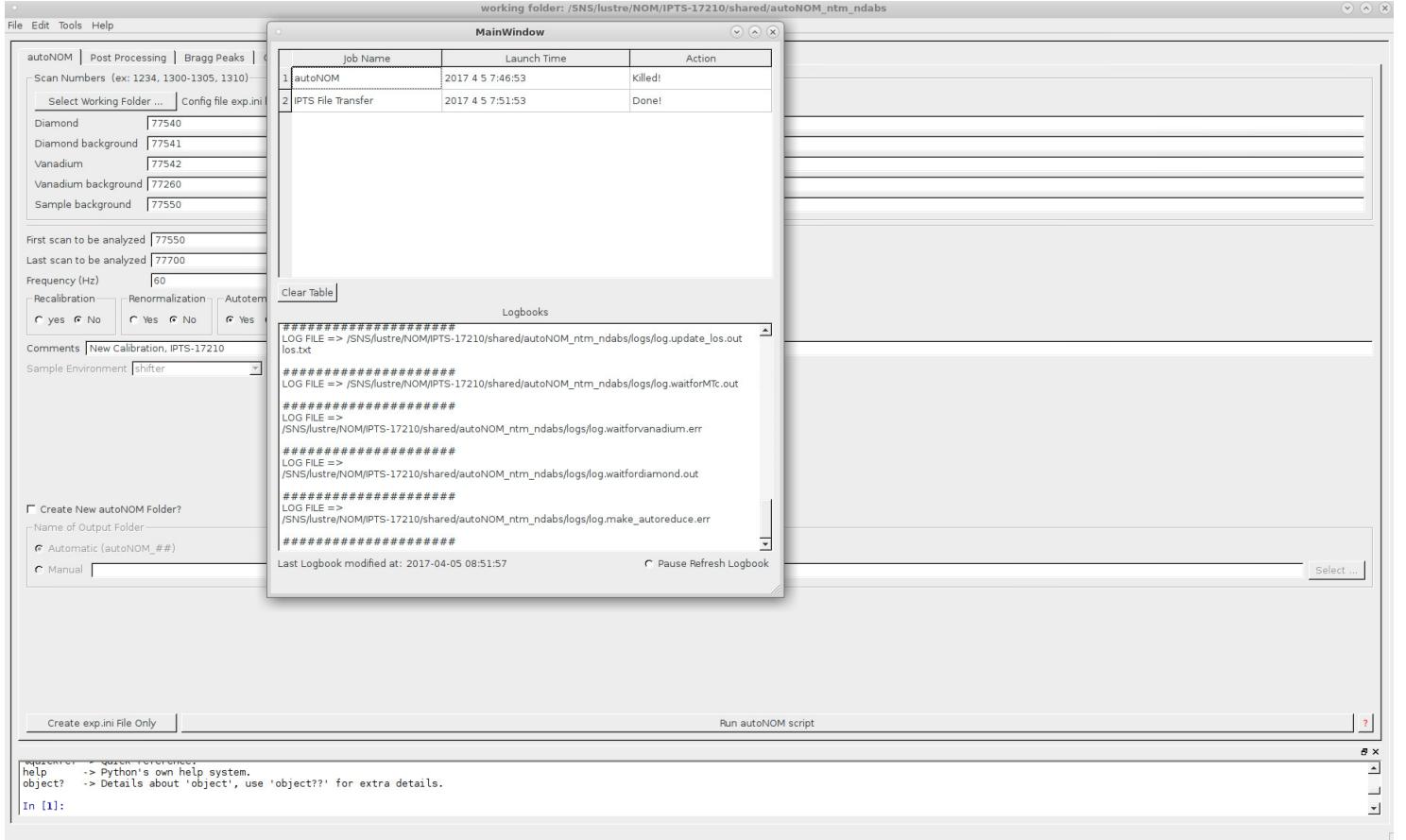
Then, press the ***autoNOM...*** button in the **Source** section to select the specific autoNOM directory. From below, you can see that an IPTS can have multiple autoNOM directories. We are selecting the autoNOM_2017A_cryostat below. Press ***Choose*** once selected:



Finally, press the **autoNOM...** button in the **Target** section to select where you will transfer the files. We are selecting the autoNOM_new_test directory below in IPTS-17210. Press **Choose** once selected:



Now, you are ready to transfer. Press the **Transfer Files** button and the transfer will start. the Job Monitor window should appear and let you know when the transfer is complete. This is usually a very quick transfer.

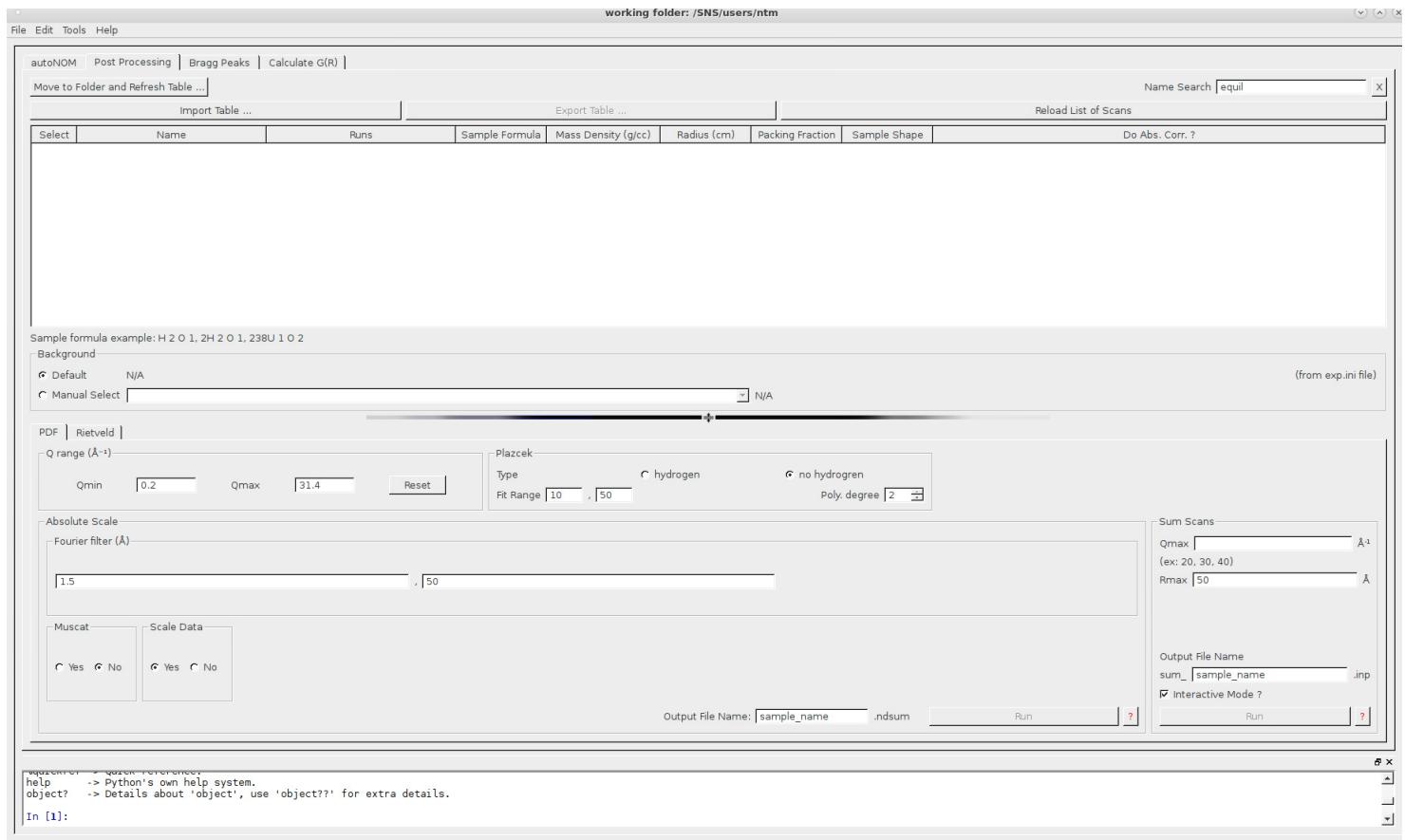


3.2 Post-Processing of runs

After we have kicked off the autoreduction and generated individual processed runs of the data, we can begin the post-processing step. Here, we can do more involved data reduction where we combine multiple runs for better statistics and data quality and perform more advanced corrections if needed.

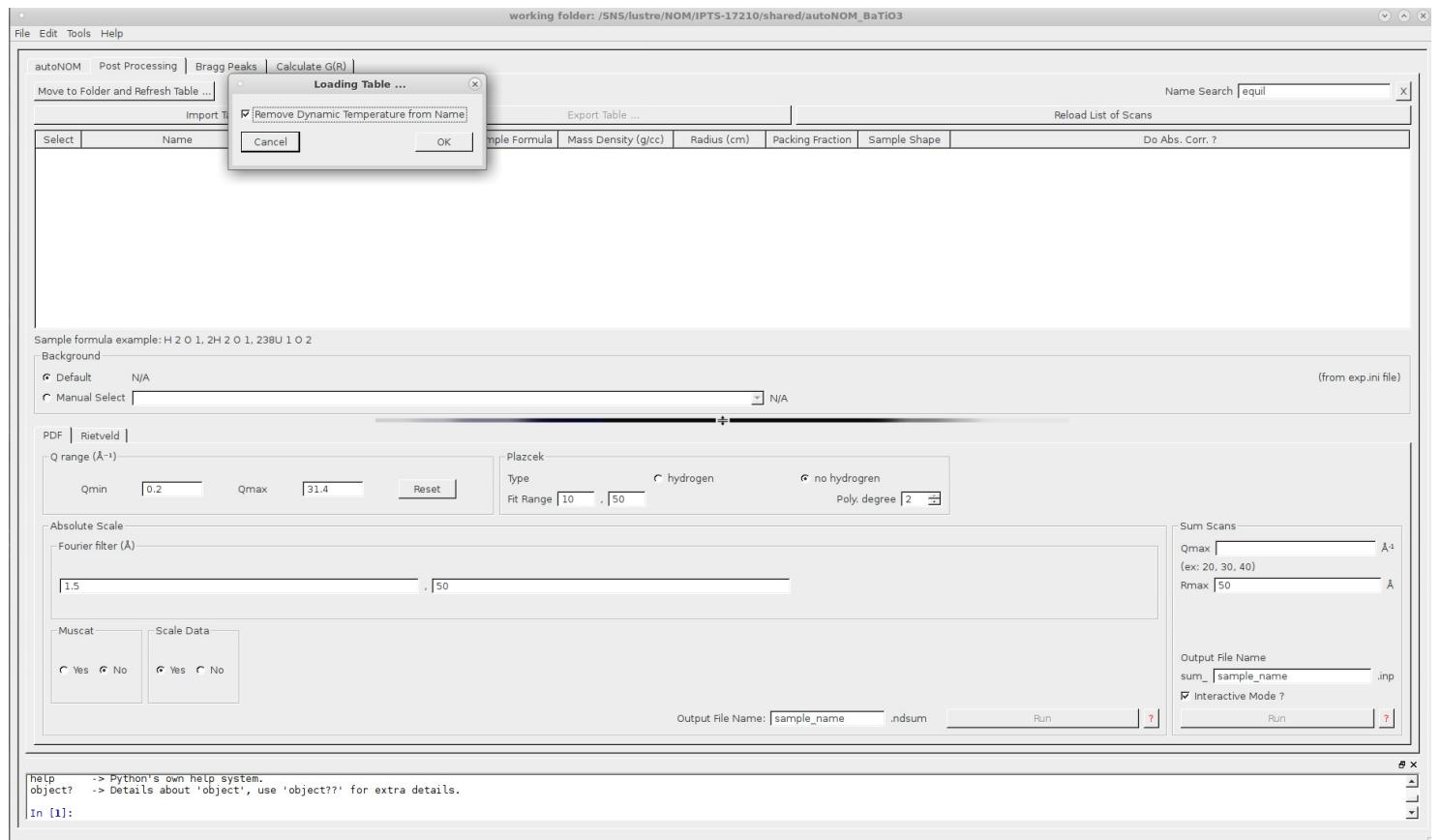
3.2.1 Load Runs into Table

Below is the ***Post-Processing*** tab:

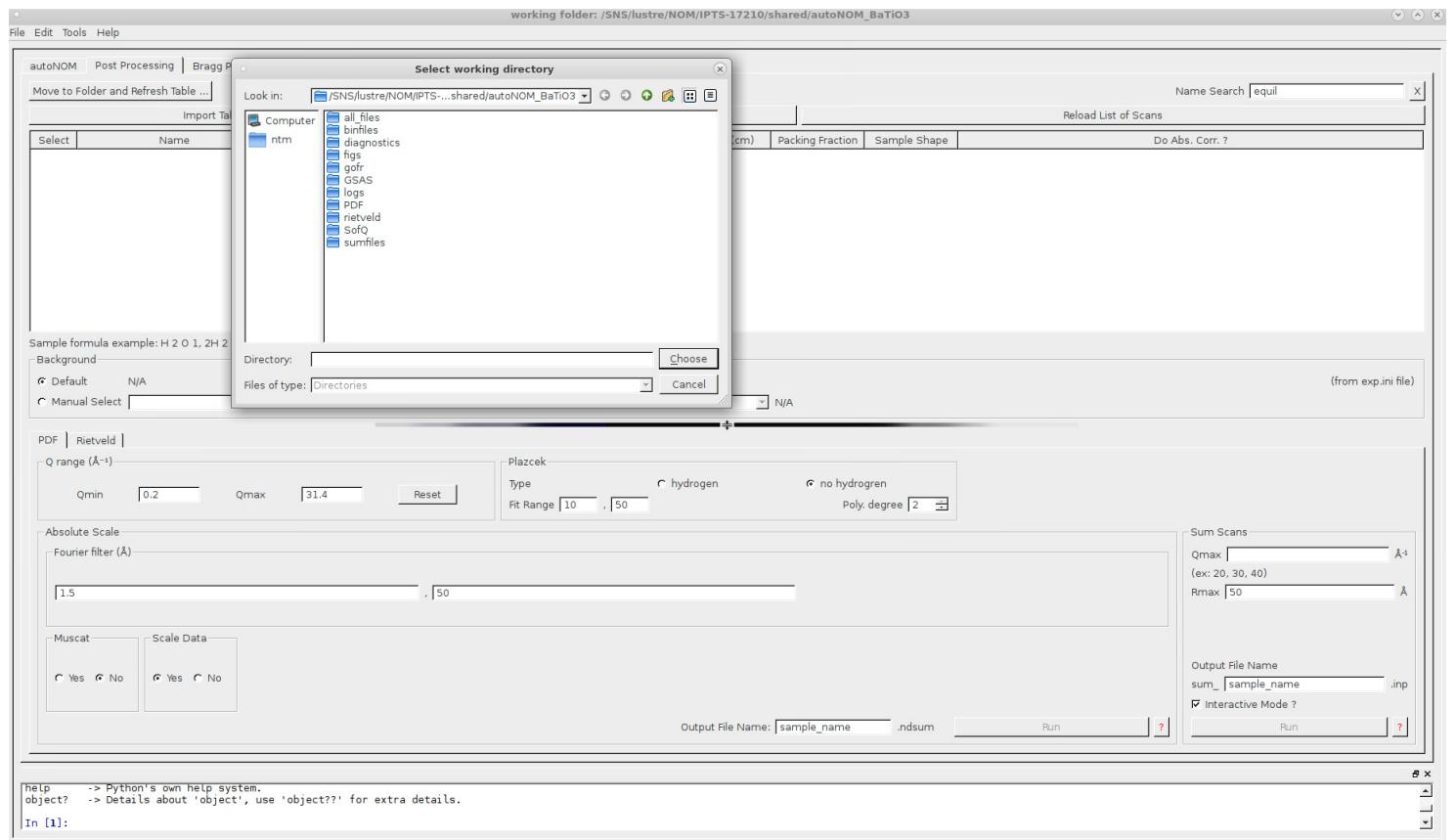


From here, we must first import our individual run information into the table. We do so by selecting the ***Move To Folder and Refresh Table...*** button. We are presented with the following dialog box asking about the Dynamic Temperature. From the individual runs, the actual temperature of the experiment is appended to the title. We can remove this from the title to group runs together in a more effect way by checking the box. You can keep this temperature in the title to split up groups of runs to exclude ones that may not be actually at the correct temperature (due to equilibration from a temperature ramp taking longer than expected) by un-checking the box. Make your selection and press

the ***Okay*** button:



Next, the file dialog box will display to choose the directory where the List of Scans file is located that we will import. There are actually two versions of the file: a space-separated version (`los.txt`) and a comma-separated version (`los.csv`). In ADDIE, we read from the comma-separated version, the `los.csv` file. Navigate to the correct autoNOM directory like below and select the ***Choose*** button.



Now, the table should be populated with your experiment runs with the individual runs grouped based on similar sample runs.

Screenshot of the autoNOM software interface showing the 'autoNOM - Post Processing' tab selected. The main window displays a table of experimental runs for BaTiO₃. The table includes columns for Select, Name, Runs, Sample Formula, Mass Density (g/cc), Radius (cm), Packing Fraction, Sample Shape, and Do Abs. Corr.?. The table shows several entries, including BaTiO₃, BaTiO₃_350K, MT_3p5_for_44CaSiO₃, MT_instrument, diamond, mt_vcan, and vanadium, all set to cylindrical shape and no absorption correction.

Below the table, there is a sample formula example: H 2 O 1, 2H 2 O 1, 238U 1 O 2. The background is set to Default. A manual selection is made for BaTiO₃ with ID 77551, which corresponds to the sample formula above. The PDF/Rietveld tab is selected, showing Q range (Å⁻¹) from 0.2 to 31.4, Plazek type, hydrogen atoms, and a fit range of 10 to 50. The absolute scale is set to Fourier filter (Å) with a value of 1.5. The sum scans section specifies Qmax at 50 Å and Rmax at 50 Å. The output file name is set to 'sum_sample_name.ndsum'. A help message in the bottom left corner indicates that 'object?' refers to Python's own help system.

If you have trouble viewing the contents of the table based on your monitor (can be an issue with laptop displays), you can use the bar shown below to shrink the post-processing options below the table:



3.2.2 Selection of Runs from Table

You can edit this table and export the changes using the **Export Table...** command. Then, when you need to import those changes into the table for another session, you can use the **Import Table...** to re-populate the table with

the saved table. The **Reload List of Scans...** button will refresh the table while an experiment is running and keep all the changes you have made. If you need to just start again, you can use the **Refresh/Reset Table...** command from the right-click options described in more detail below.

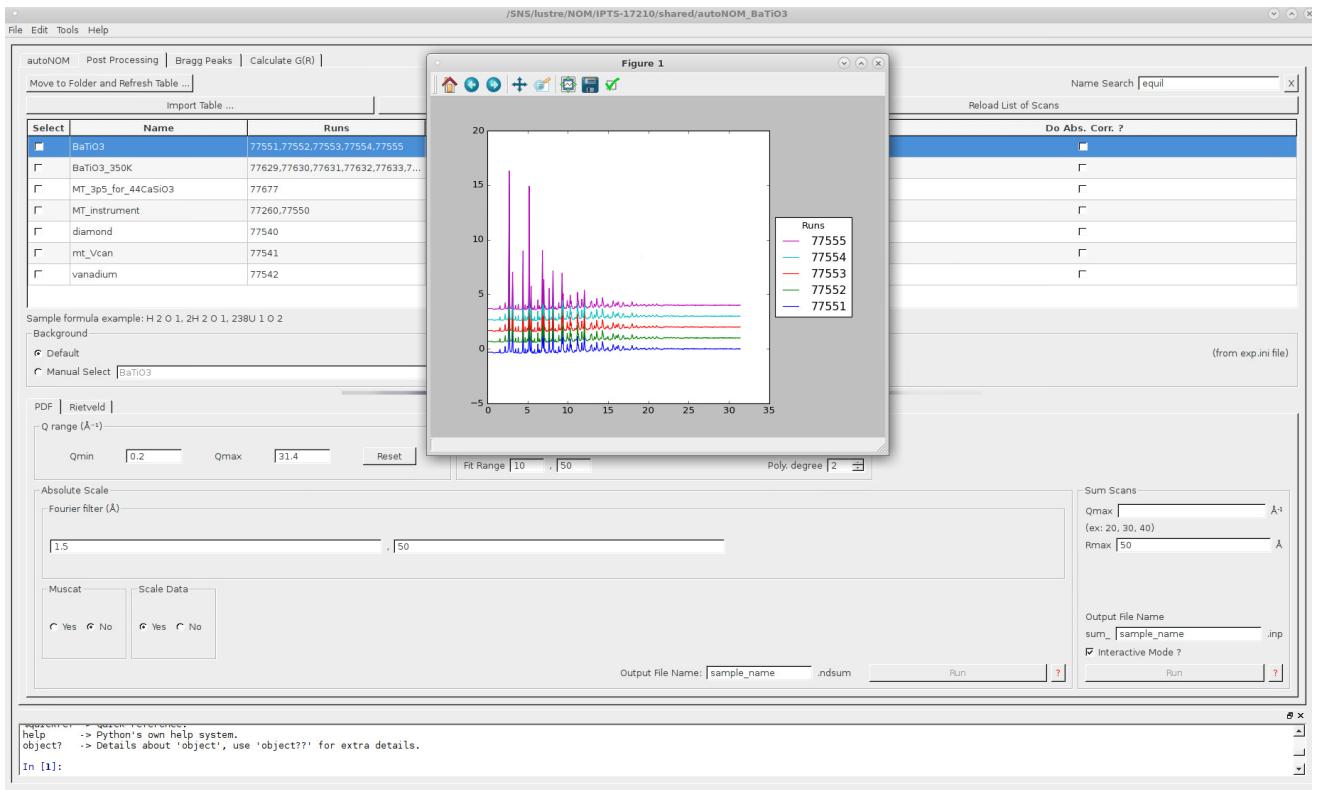
To edit any of the fields in the table, you can just double click and input any information you would like. This includes changing the name of the group or deleting runs for a given row. You can select multiple rows by holding the *Ctrl* button for individual selections or holding down *Shift* to chose a range of rows. You can right-click to get options for individual rows as well.

The screenshot shows the autoNOM software interface with the following details:

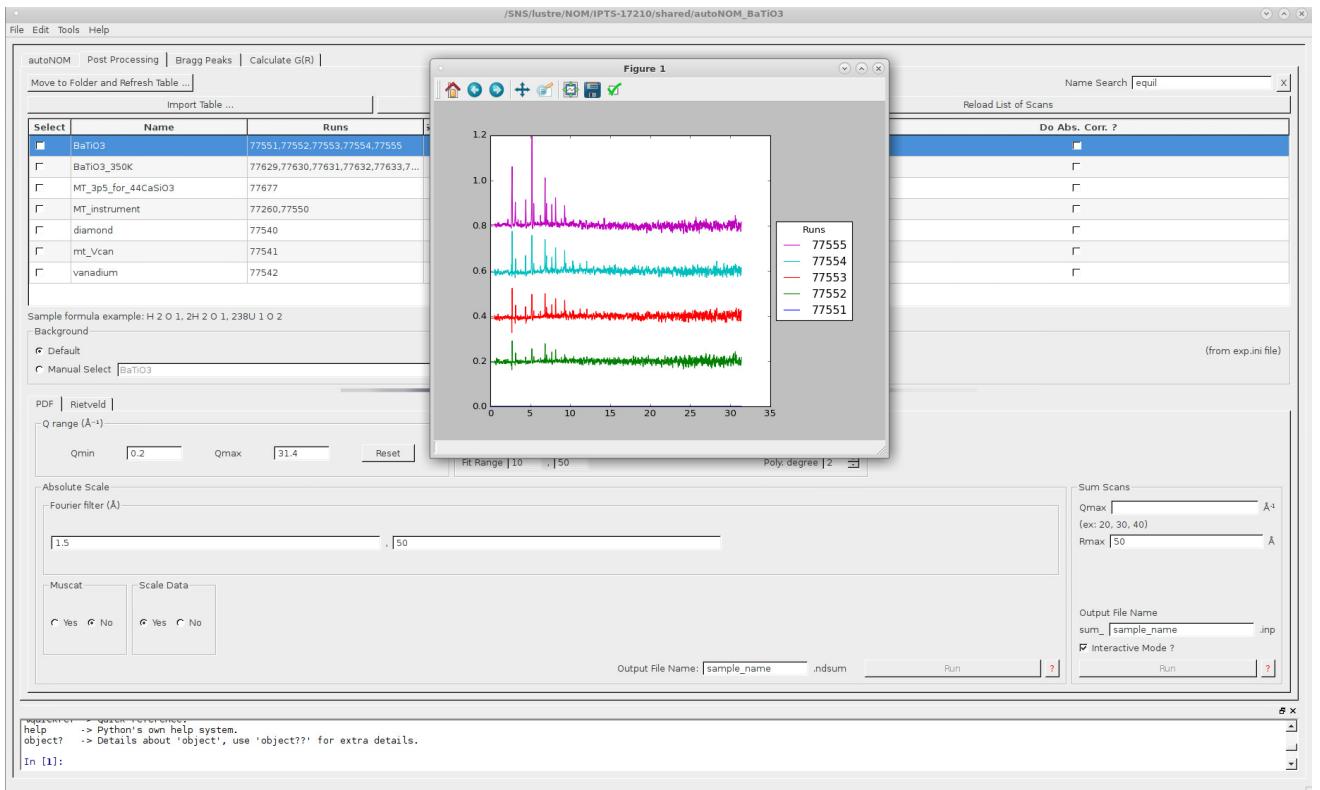
- Top Bar:** File, Edit, Tools, Help, /SNS/lustre/NOM/IPTS-17210/shared/autoNOM_ntm_ndabs
- Toolbar:** autoNOM, Post Processing, Bragg Peaks, Calculate G(R), Move to Folder and Refresh Table ...
- Table:** A grid of experimental runs with columns: Select, Name, Runs, sample formula, Mass Density (g/cc), Radius (cm), Packing Fraction, Sample Shape, and Do Abs. Corr. ?.
- Context Menu (Right-clicked on BaTiO3 row):**
 - Undo
 - Redo
 - Copy
 - Paste
 - Clear
 - Check All
 - Unchecked All
 - Inverse Selection
 - Insert Blank Row
 - Duplicate Row
 - Remove Row(s)
- Buttons:** Import Table ..., Export Table ..., Reload List of Scans, Name Search equil.
- Plot Area:** Shows a plot of Intensity vs. Q-range (Å⁻¹) with a peak labeled "BaTiO3".
- Plot Options:** Plot, Plot Diff (1st run), Plot Diff (Avg.), Refresh/Reset Table, Clear Table.
- Absolute Scale:** Fourier filter (Å⁻¹) set to 1.5, Muscat, Scale Data, Type (radio buttons: hydrogen, no hydrogen), Fit Range [10, 50], Poly. degree [2].
- Sum Scans:** Sum Scans, Qmax [50] Å⁻¹, Rmax [50] Å.
- Output:** Output File Name: sample_name.nsdum, Run, Interactive Mode? (checkbox checked).
- Bottom:** In [1]: Python help text.

These options are as follows:

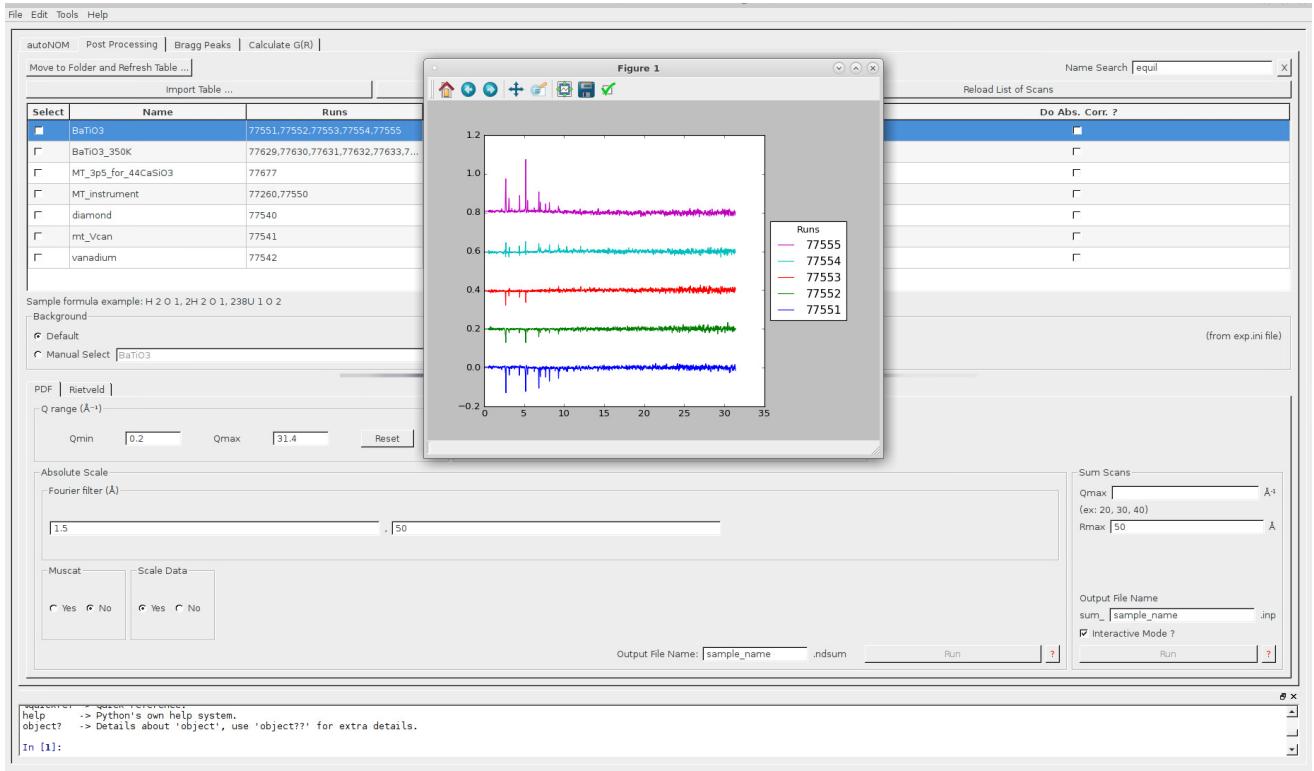
- ***Undo***: Undo the last action in the table.
- ***Redo***: Redo the last undone action in the table.
- ***Copy***: Copy the selected contents of a field in a row.
- ***Paste***: Paste copied contents in a field of a row.
- ***Clear***: Clear the contents of a field in a row.
- ***Check All***: Check all of the **Select** boxes for all rows.
- ***Unchecked All***: Uncheck all of the **Select** boxes for all rows.
- ***Inverse Selection***: Reverse the selection of the rows. Changes checked rows to unchecked rows and vice versa.
- ***Insert Blank Row***: Insert an new, blank row.
- ***Duplicate Row***: Duplicate an entire row in the table based on selection.
- ***Remove Row(s)***: Remove an entire row or rows based on selection.
- ***Plot***: Plot the $S(Q)$ for individual runs on the same plot (with an 0.2 offset on the y-axis). If the data has not finished processing or the $S(Q)$ does not exists, it will not show up in the graph. An example is shown below:



- **Plot Diff (1st run)....:** Plot the difference in $S(Q)$ for individual runs on the same plot (with an 0.2 offset on the y-axis) using the 1st listed run as the reference. If the data has not finished processing or the $S(Q)$ does not exist, it will not show up in the graph. The run subtracted is the first run plotted and shows up as a horizontal line at 0 on the y-axis. An example is shown below:



- **Plot Diff (Avg.)....:** Plot the difference in $S(Q)$ for individual runs on the same plot (with an 0.2 offset on the y-axis) using the average of the runs as the reference. If the data has not finished processing or the $S(Q)$ does not exist, it will not show up in the graph. An example is shown below:



- **Refresh/Reset Table:** Reloads the table with the current List of Scans file (los.csv)

- **Clear Table....:** Removes all contents from the table.

You can add sample information into the table by editing the necessary fields. Below is an example for the barium titanate where the sample formula, mass density, radius of the sample can, and packing fraction have been input for the given row:

The screenshot shows the autoNOM software interface with the following details:

- Table of Runs:**

Select	Name	Runs	Sample Formula	Mass Density (g/cc)	Radius (cm)	Packing Fraction	Sample Shape	Do Abs. Corr. ?
<input checked="" type="checkbox"/>	BaTiO ₃	77551,77552,77553,77554,77555,7...	Ba Ti O 3	6.02	.6	0.7]	cylindrical	<input type="checkbox"/>
<input type="checkbox"/>	BaTiO ₃ _350K	77629,77630,77631,77632,77633,7...					cylindrical	<input type="checkbox"/>
<input type="checkbox"/>	MT_3p5_for_44CaSiO ₃	77677					cylindrical	<input type="checkbox"/>
<input type="checkbox"/>	MT_instrument	77260,77550					cylindrical	<input type="checkbox"/>
<input type="checkbox"/>	diamond	77540					cylindrical	<input type="checkbox"/>
<input type="checkbox"/>	mt_Vcan	77541					cylindrical	<input type="checkbox"/>
<input type="checkbox"/>	vanadium	77542					cylindrical	<input type="checkbox"/>
- Search and Export:** Includes "Name Search" (equil), "Import Table ...", "Export Table ...", and "Reload List of Scans".
- Background Selection:** Options for "Default" or "Manual Select" (set to mt_Vcan).
- Processing Parameters:**
 - PDF | Rietveld
 - Q range (Å⁻¹): Qmin [0.2], Qmax [31.4], Reset
 - Plazek: Type [hydrogen], Fit Range [10, 50], Poly. degree [2]
 - Absolute Scale: Fourier filter (Å): 1.5, 50
 - Muscat: Scale Data: Yes/No
 - Sum Scans: Qmax [A⁻¹], Rmax [50 Å]
 - Output File Name: BaTiO₃.ndsum, Run, ?
 - Interactive Mode? Run, ?
- Help:** Quickref, help, object?

Once the table is in a good state, we are ready to begin post-processing for a given set of runs. We have already covered the options available for selecting runs based on the right-click options. You will need to have the **Select** checkbox ticked for all rows that you want to use for post-processing.

One tool that may also be of use is the **Name Search** in the top right part of the tab. This allows you to select scans that match part of what you input into the field. Below, we show the BaTiO₃ and BaTiO₃_350K rows that were selected based on a match with the "BaTi" input in the **Name Search**.

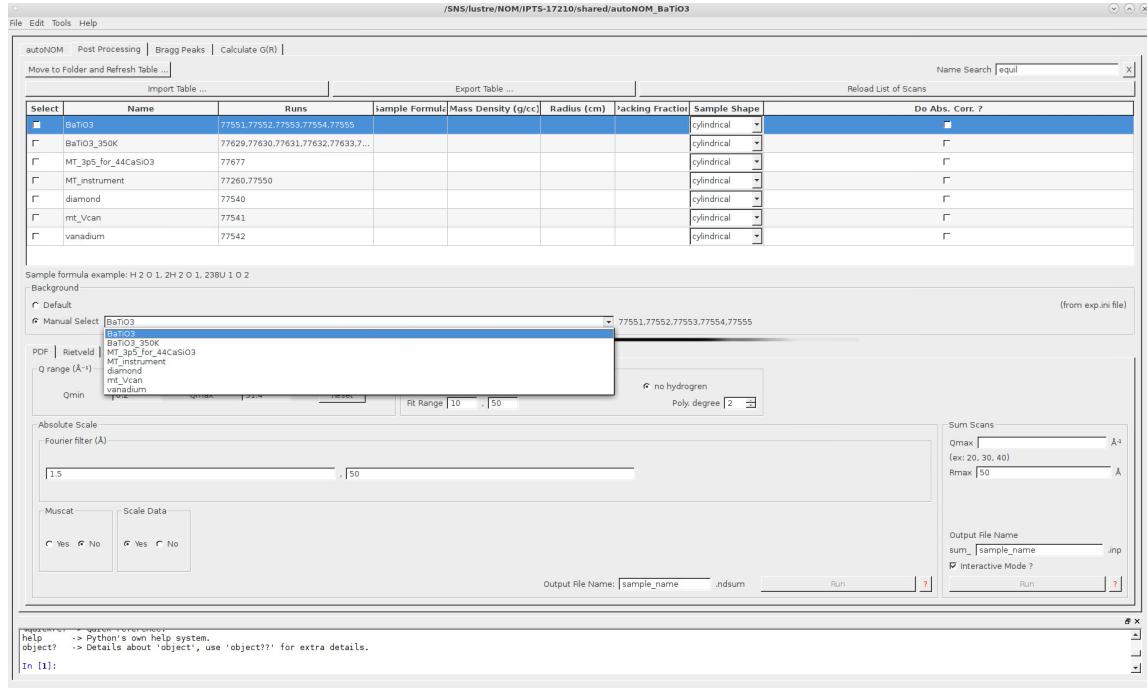
The screenshot shows a software window titled "autoNOM Post Processing | Bragg Peaks | Calculate G(R) | /SNS/lustre/NOM/IPTS-17210/shared/autoNOM_BaTiO3". The main area is a table with the following data:

Select	Name	Runs	Sample Formula	Mass Density (g/cc)	Radius (cm)	Tacking Fraction	Sample Shape	Do Abs. Corr. ?
<input checked="" type="checkbox"/>	BaTiO3	77551,77552,77553,77554,77555,7...					cylindrical	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	BaTiO3_350K	77629,77630,77631,77632,77633,7...					cylindrical	<input checked="" type="checkbox"/>
<input type="checkbox"/>	MT_3p5_for_44CaSiO3	77677					cylindrical	<input type="checkbox"/>

This feature can help in selecting runs but also deleting unneeded runs. For example, if you have performed a temperature ramp and named the title of those runs "Ramp...", you can do a **Name Search** to select those rows and then delete them via the right-click option.

3.2.3 Setting up and launching Post-Processing

After the desired rows are selected, you can now set up the post-processing options. First, we begin by specifying the multiple background files to be subtracted from the data in the **Background** section. These are typically your empty container runs (i.e. vanadium cans, capillaries, NMR tubes). The **Default** will be the single empty container run that was used for the individual runs during the autoreduction. **Manual select** will give you the option to select from one of the rows in the table. The run numbers for that row will be displayed beside this drop-down box. Any changes you make to the row in the table (change name, add/subtract run numbers) will be reflected for this drop-down and the runs displayed.



From here, there are two tabs to select from:

- **PDF**: Used for summing scans together and applying other corrections. Will produce Bragg profile and total scattering files. Uses autoNOM data reduction to perform the post-processing.
- **Rietveld**: Used for summing scans. Will produce Bragg profile files. Uses Mantid data reduction to perform the post-processing (specifically, the [SNSPowderReductionscript](#)).

PDF Tab

On the **PDF** tab, we have two separate programs that can be launched: **Sum Scans** and **Absolute Scale**. The ***Q* range** and ***Plazcek*** are sections that is common to both.

- ***Q range***: In this section, we can adjust Q_{min} and Q_{max} , which are the minimum and maximum Q to use for the Fourier transform, respectively.
- ***Plazcek***: In this section, we can select different hydrogen corrections and polynomial fits to the data and the range over which the correction is applied.

The ***hyrdogen*** button selects the correction that is described in Equation 2.2 under $hyd=2$ which is applied to Equation 2.6.

The ***no hyrdogen*** button selects the polynomial described in Equation 2.2 under $hyd=0$ which is applied to Equation 2.6 with the degree of the polynomial chosen based on the value in the ***Poly. degree*** field.

The ***Fit Range*** gives the limits in Q for these least-square fits for S(Q).

- ***Sum Scans***: This is the driver for summing individual runs together.

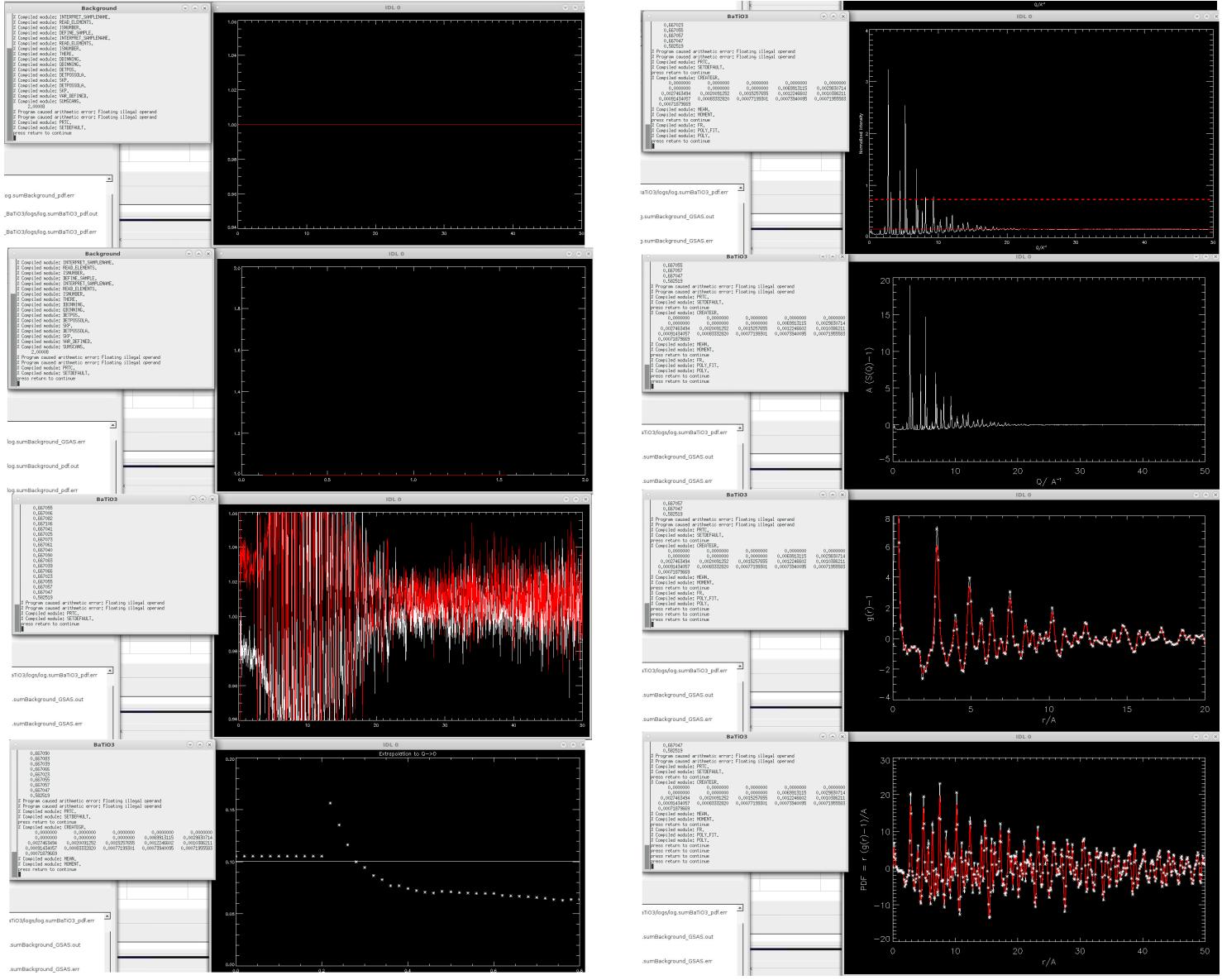
Qmax allows for a list to use for the summed S(Q) datasets, where a simple truncation is performed.

Rmax specifies how far out in real-space the pair distribution function will be calculated.

Output File Name is just the name for the input file generated to run the ***Sum Scans*** program externally.

For ***Interacive Mode?***, when we run ***Sum Scans***, the external program produces diagnostic plots launched in x-terminals. If the ***Interacive Mode?*** is selected, these plots will be displayed and the User must press **Enter** when finished looking at the plots. If the User does not wish to view the plots and let the program run "silently", uncheck the box before running.

An example of these plots are shown below:



- **Absolute Scale** This is the driver for performing multiple scattering corrections and also to put the data on a absolute scale given the necessary information in the table.

Fourier filter: Specifies the real-space range for $G(r)$ over which to

apply a Fourier filter. This allows for "cropping" the real-space data by performing the reverse transform back to reciprocal space on the data outside the filter range, subtracts this reverse transform from the $S(Q)$, and then transforms this $S(Q)$ back to real-space $G(r)$ with only the region specified by the Fourier filter.

Muscat: Applies a multiple scattering absorption correction to the data based on both the sample material information and the geometry of the container specified in the table.

Scale Data: Re-scales the data to a theoretical $Q \rightarrow \infty$ based on the sample density and packing fraction.

Rietveld Tab

From the **Rietveld** Tab, we can launch Mantid to also sum together runs and produce diffraction data. This mainly drives the **SNSPowderReduction** algorithm found in Mantid used by other powder diffractometers at the SNS. Currently, the $S(Q)$ and $G(r)$ are not produced by this tab but is a work in progress. The **Rietveld** Tab is shown below:

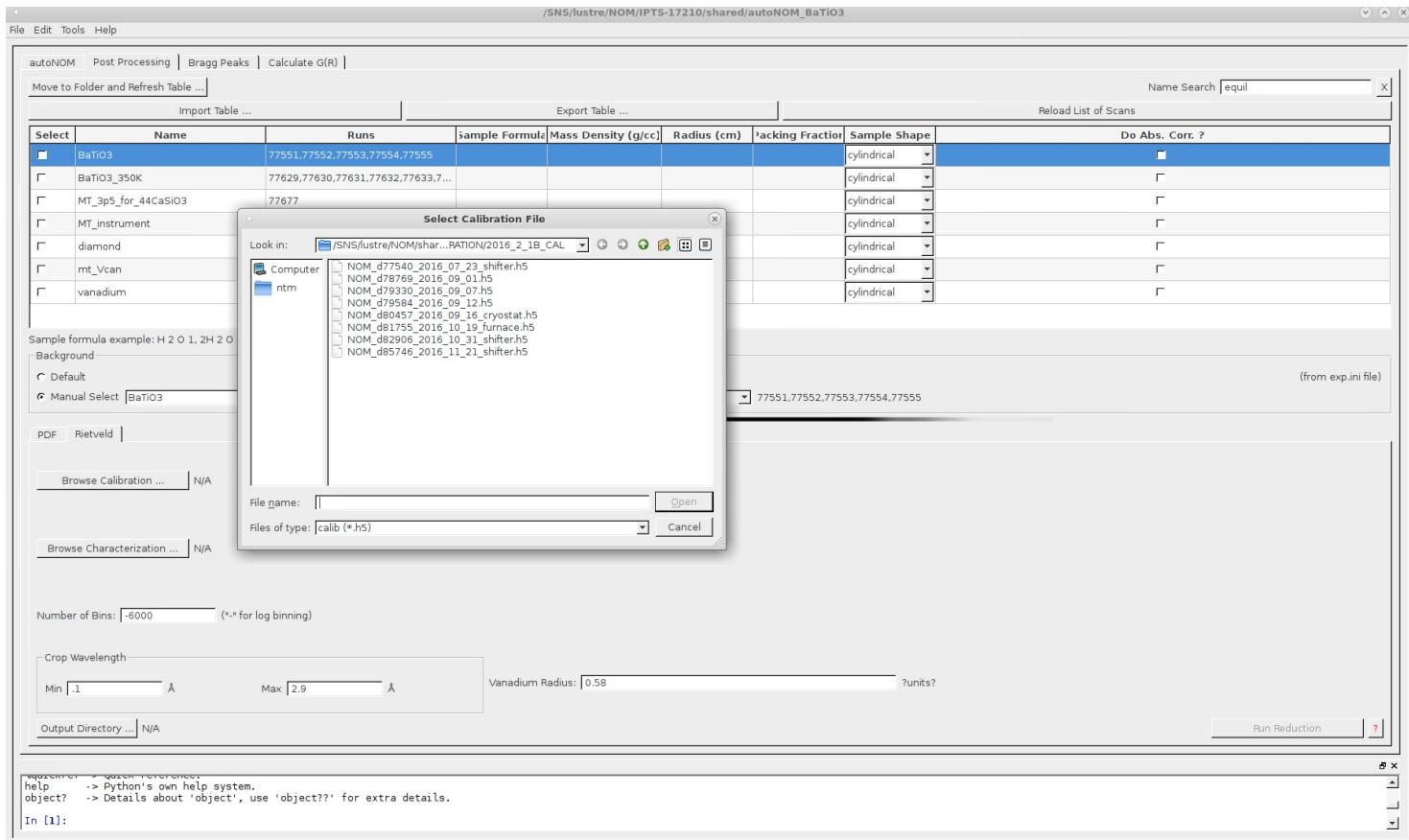
The screenshot shows the autoNOM software interface with the following details:

- Top Bar:** File, Edit, Tools, Help, /SNS/lustre/NOM/IPTS-17210/shared/autoNOM_BaTiO3
- Toolbar:** AutoNOM, Post Processing, Bragg Peaks, Calculate G(R), Move to Folder and Refresh Table ..., Import Table ..., Export Table ..., Name Search [equil], Reload List of Scans.
- Table:** A grid showing experimental runs. The columns are Select, Name, Runs, Sample Formula, Mass Density (g/cc), Radius (cm), Packing Fraction, Sample Shape, and Do Abs. Corr.?

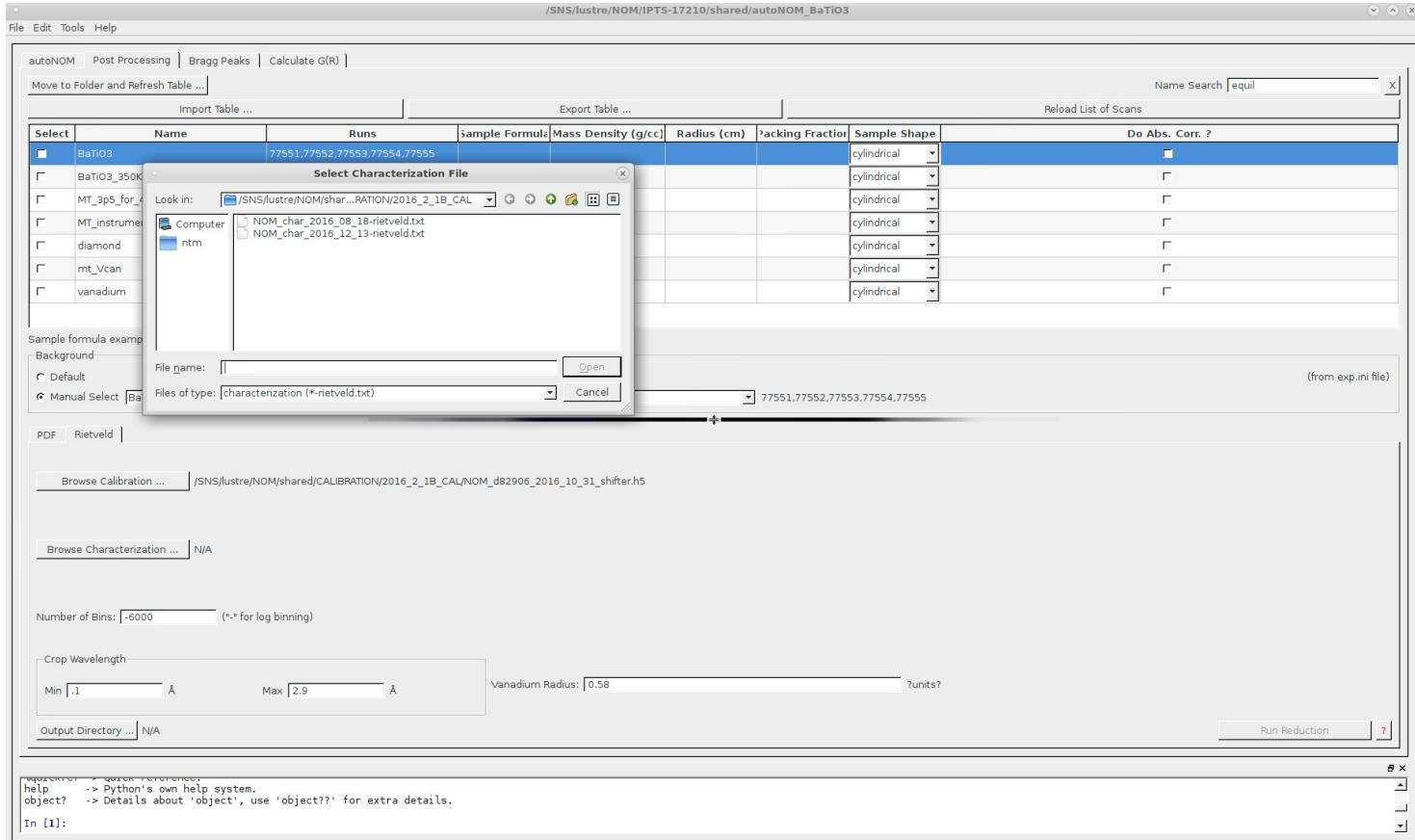
Select	Name	Runs	Sample Formula	Mass Density (g/cc)	Radius (cm)	Packing Fraction	Sample Shape	Do Abs. Corr.?
<input checked="" type="checkbox"/>	BaTiO3	77551,77552,77553,77554,77555				cylindrical	<input checked="" type="checkbox"/>	
<input type="checkbox"/>	BaTiO3_350K	77629,77630,77631,77632,77633,7...				cylindrical	<input type="checkbox"/>	
<input type="checkbox"/>	MT_3p5_for_44CaSiO3	77677				cylindrical	<input type="checkbox"/>	
<input type="checkbox"/>	MT_instrument	77260,77550				cylindrical	<input type="checkbox"/>	
<input type="checkbox"/>	diamond	77540				cylindrical	<input type="checkbox"/>	
<input type="checkbox"/>	mt_Vcan	77541				cylindrical	<input type="checkbox"/>	
<input type="checkbox"/>	vanadium	77542				cylindrical	<input type="checkbox"/>	
- Text Fields:** Sample formula example: H 2 O 1, 2H 2 O 1, 238U 1 O 2, Background: Default, Manual Select: BaTiO3 (from exp.ini file).
- Buttons:** PDF, Rietveld, Browse Calibration ..., Browse Characterization ..., Output Directory ...
- Inputs:** Number of Bins: 6000 (* for log binning), Crop Wavelength: Min .1 Å, Max 2.9 Å, Vanadium Radius: 0.58 Å, ?units?, Run Reduction, In [1]:
- Help:** Python's own help system, Details about 'object', use 'object??' for extra details.

To launch the post-processing data reduction from this tab, you need to do the following:

- **Browse Calibration...:** First, you need to select the appropriate calibration file to use. Press the **Browse Calibration...** button to browse the calibration files available commonly shared to all NOMAD Users. Select one that is the most recent with the same sample environment that your experiment is using. You will see something similar to the selection below:

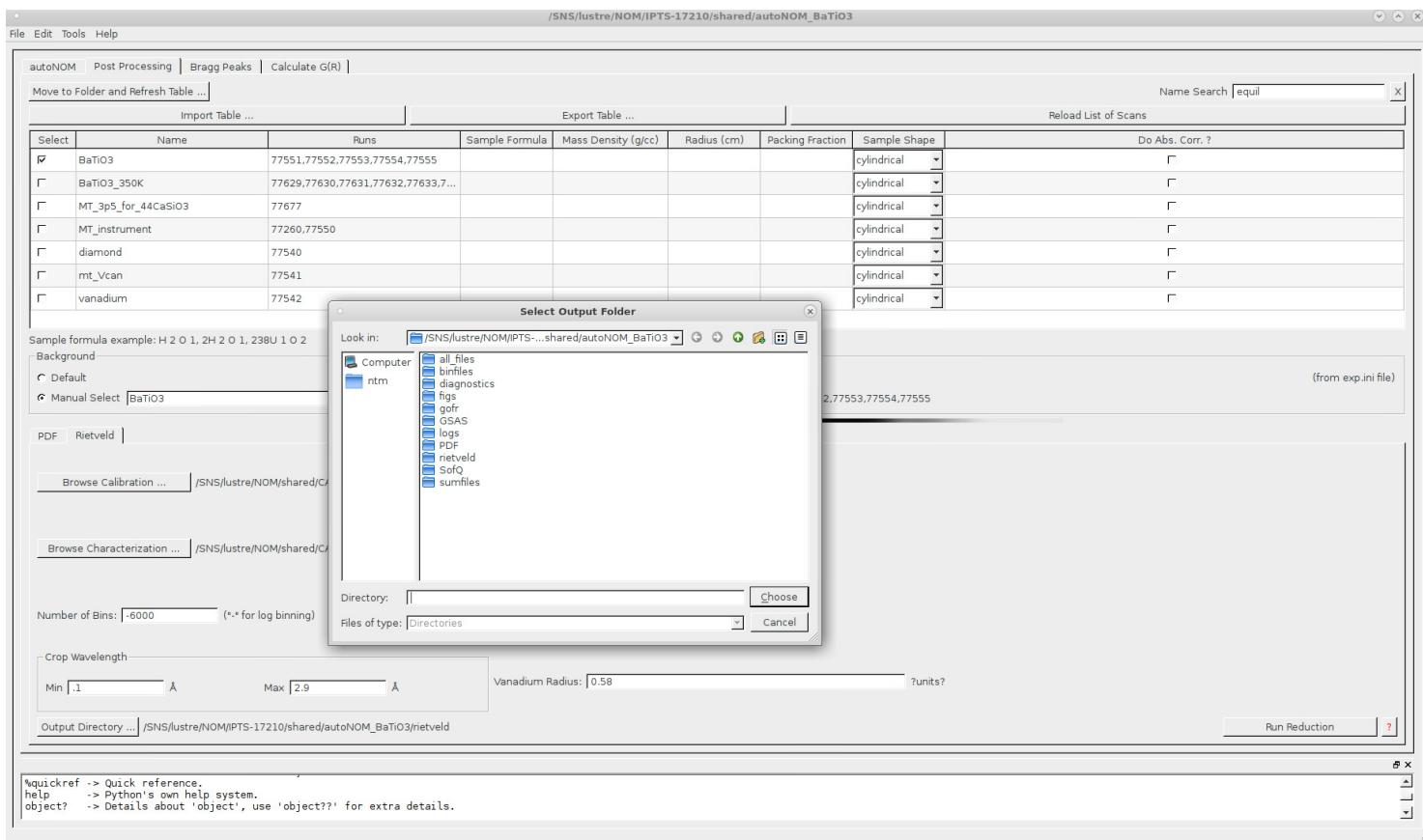


- **Browse Characterization...:** Next, you must also select a characterization file for the instrument. Press the **Browse Characterization...** button to browse the characterization files available commonly shared to all NOMAD Users. Select one that is the most recent. You will see something similar to the selection below:

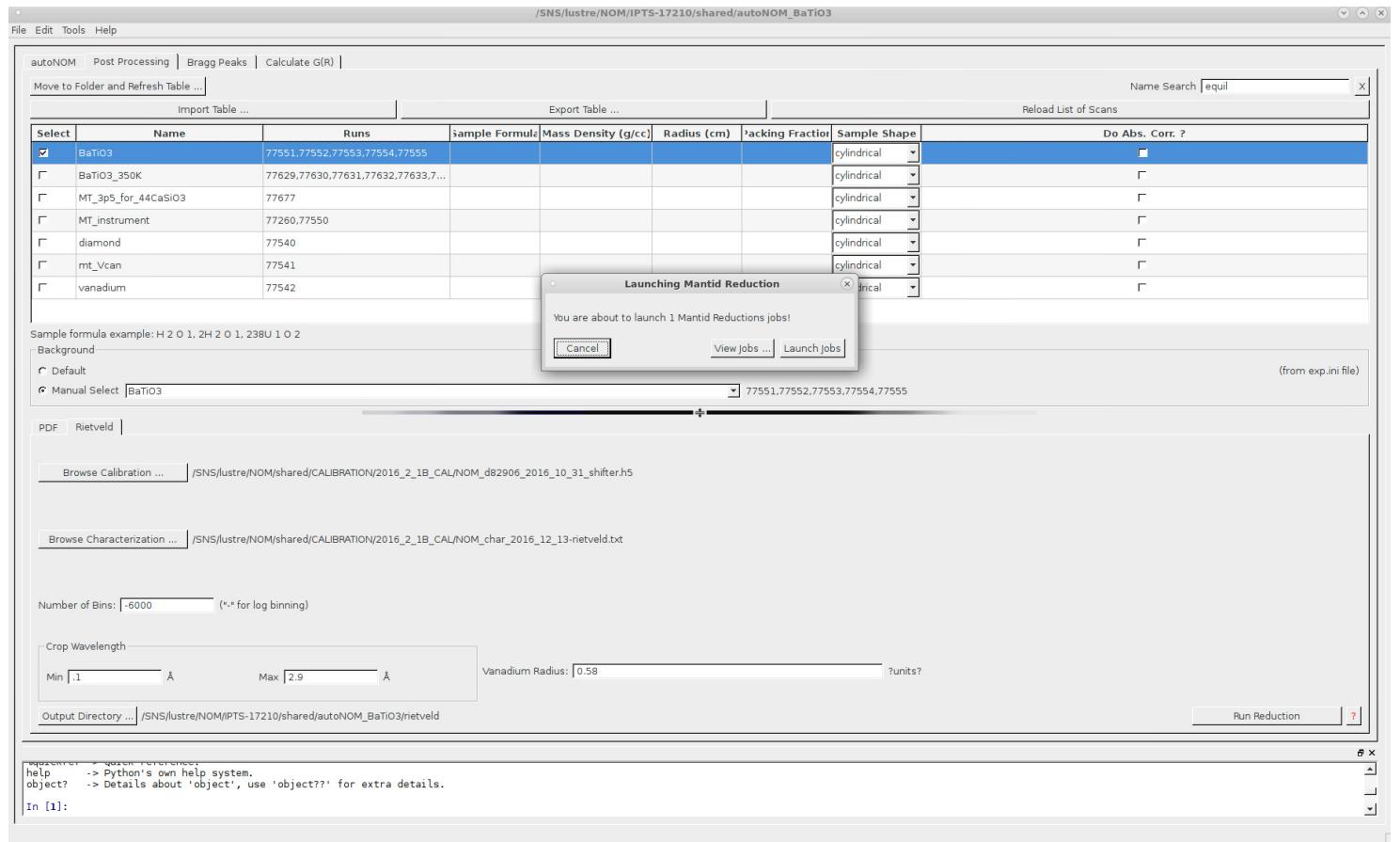


- **Number of Bins:** This defines the number of bins used along the x-axis. A negative value implies logarithmic binning, using the formula $x_{i+1} = x_i(1 + |\Delta x_i|)$. More detail can be found [here](#).
- **Crop Wavelength:** Specify the minimum and maximum wavelength used to crop the TOF data. This data can also be found in the characterization file but can be overridden by the values specified here.
- **Vanadium Radius:** Specify the radius of the empty vanadium can container. This is used for applying the multiple scattering absorption correction.
- **Output Directory:** This is used to specify under which directory the

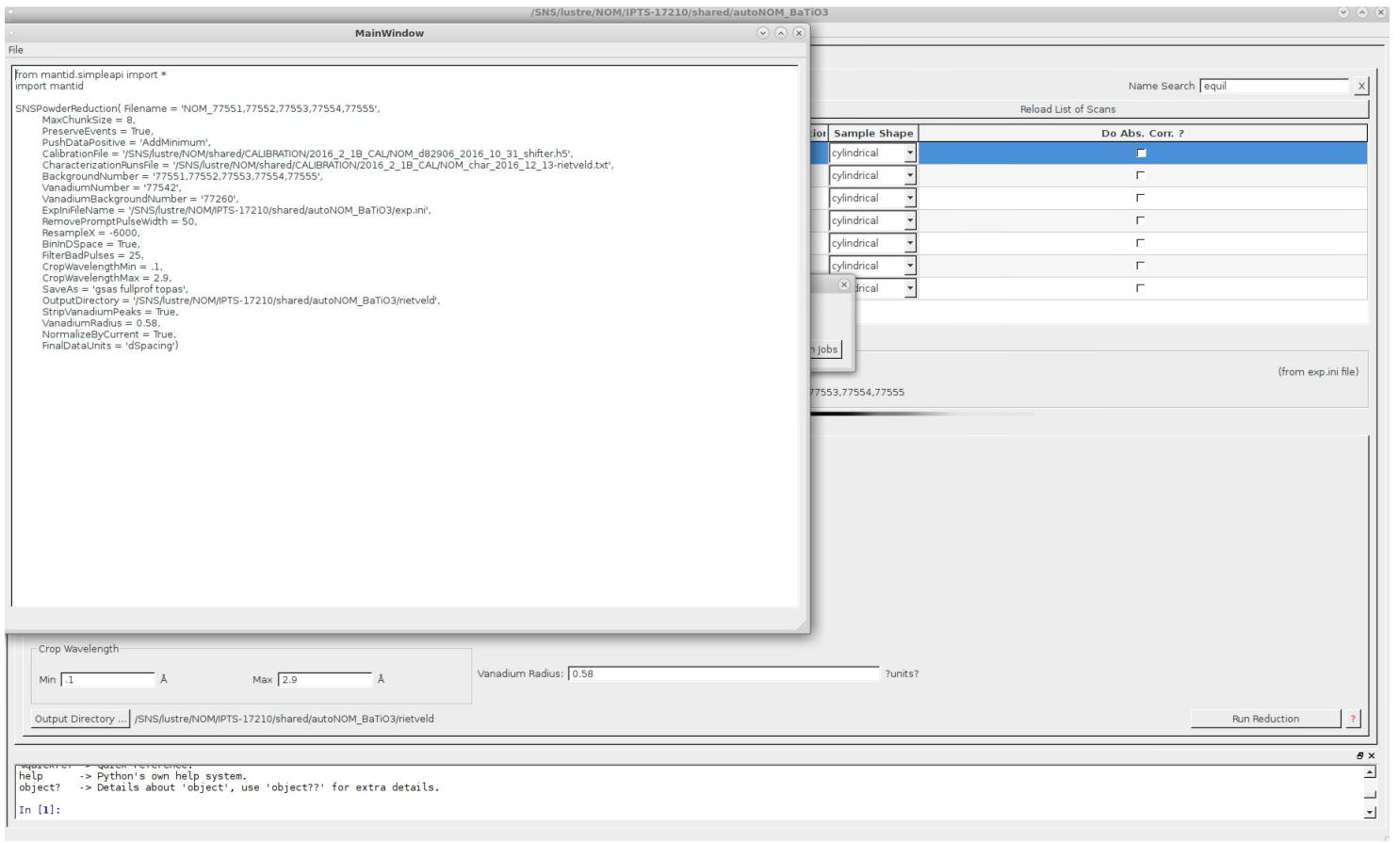
output directory will be placed. The directory will be named `rietveld` by default. It is recommended to place it inside the `autoNOM` directory or the parent `shared`. When you press the ***Output Directory*** button, you will be shown a file dialog box similar to the one below. we have already chosen the `autoNOM_BaTiO3` directory below and the output directory is displayed beside the ***Output Directory*** button:



Now, once you have selected the rows that you would like to perform Mantid post-processing data reduction on, you can press the ***Run Reduction*** button. As before, if the button is greyed out, you can select the **?** box to see what is missing for the button to activate. When you press the ***Run Reduction*** button, you will be presented with the file dialog below:



You can select **View Jobs...** to inspect the Mantid script that will be launched, similar to the one displayed below:



If everything is ready, you can select ***Launch Jobs*** to begin.

3.3 Visualize Bragg Diffraction

3.3.1 Load Bragg data

3.3.2 Adjust Graphs

3.4 Visualize $S(Q)$ and $G(r)$

3.4.1 Load $S(Q)$ data

3.4.2 Adjust $S(Q)$ graphs

3.4.3 Load $G(r)$ data

3.4.4 Optimize $G(r)$

3.4.5 Adjust $G(r)$ graphs

3.4.6 Output $G(r)$