

# ADDIE User Manual

*ADvanced DIffraction Environment*

Data reduction software for NOMAD

May 2, 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

# Quick Start Guide

Add abbreviated startup guide to this section. Distill what is in the rest of the manual

## Chapter 4

# 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

## 4.1 Launch automatic data reduction of individual runs

### 4.1.1 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

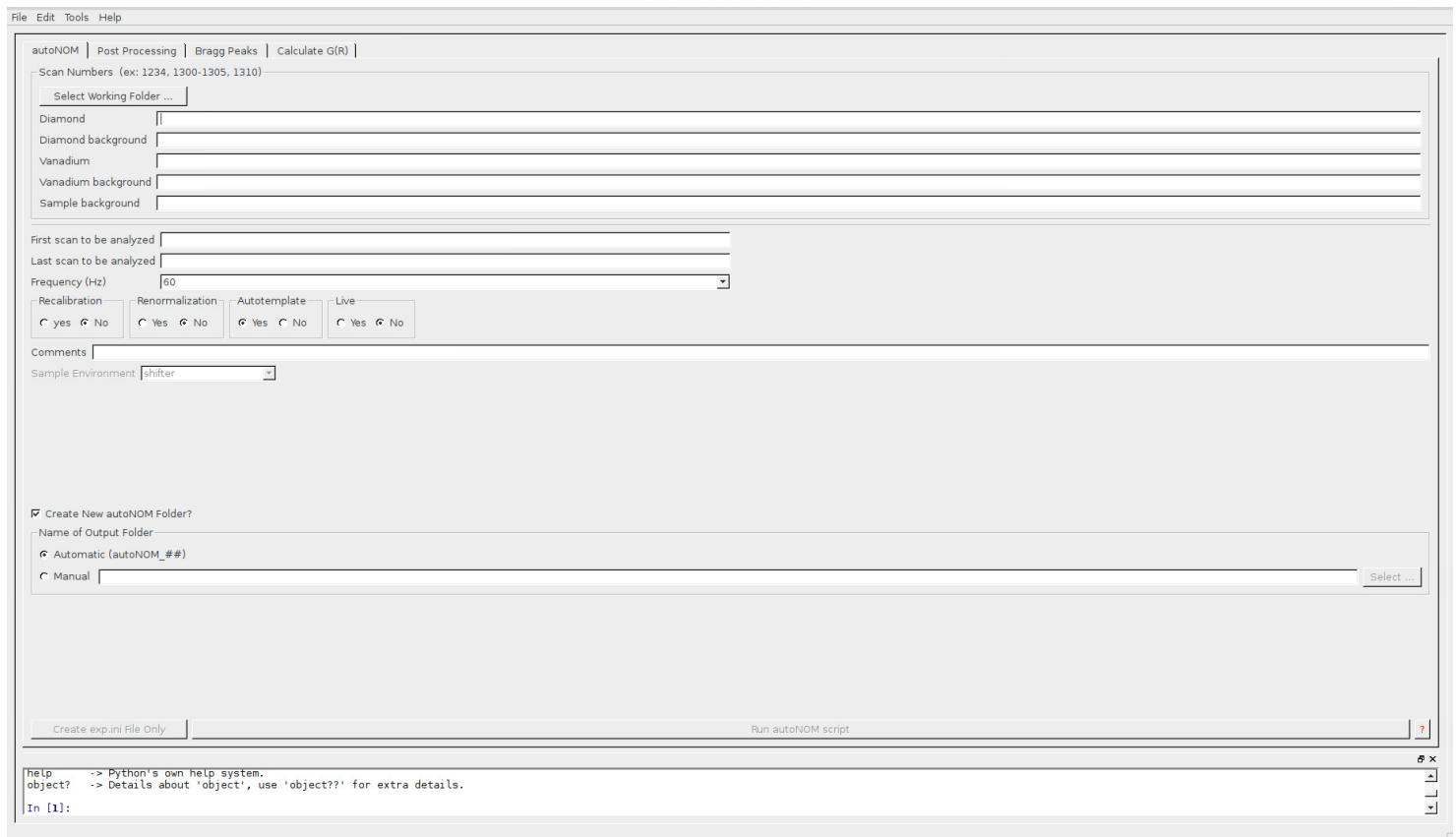
You can examine the NeXus files from the command line of a terminal using `nxbrowse <NeXus filename>`. These files have a directory structure. You can `ls` to list the current level of the directory and use `cd` to enter a directory. All these files have the `entry` as the initial entry point. Then, 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.

#### 4.1.2 Experiment Information Input

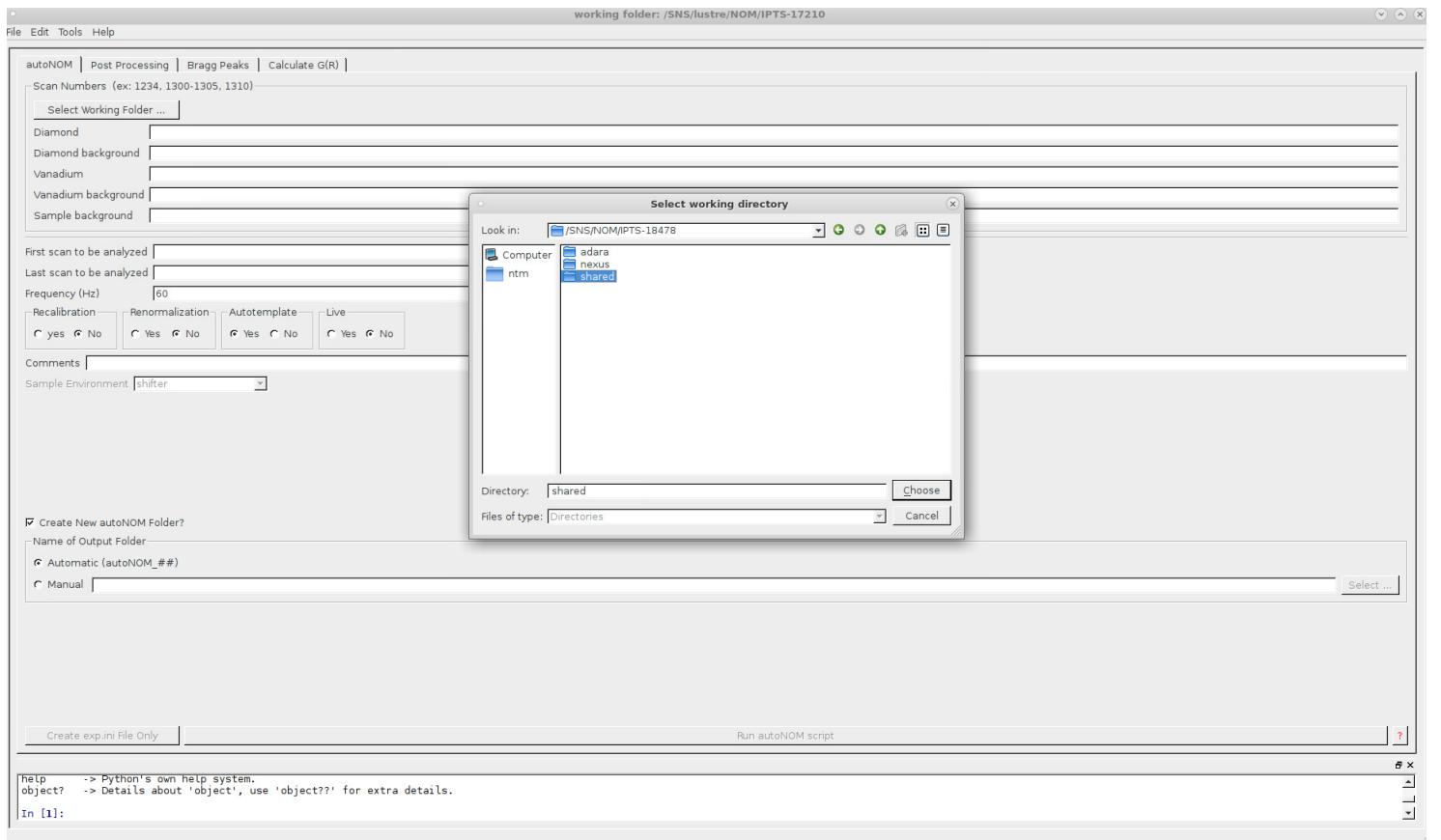
ADDIE can be used to launch an automated data reduction, or autoreduction, of your sample runs as they complete and produce NeXus files. The autoreduction processes the NeXus files as they appear under your IPTS folder.

#### Loading In the Experiment Information

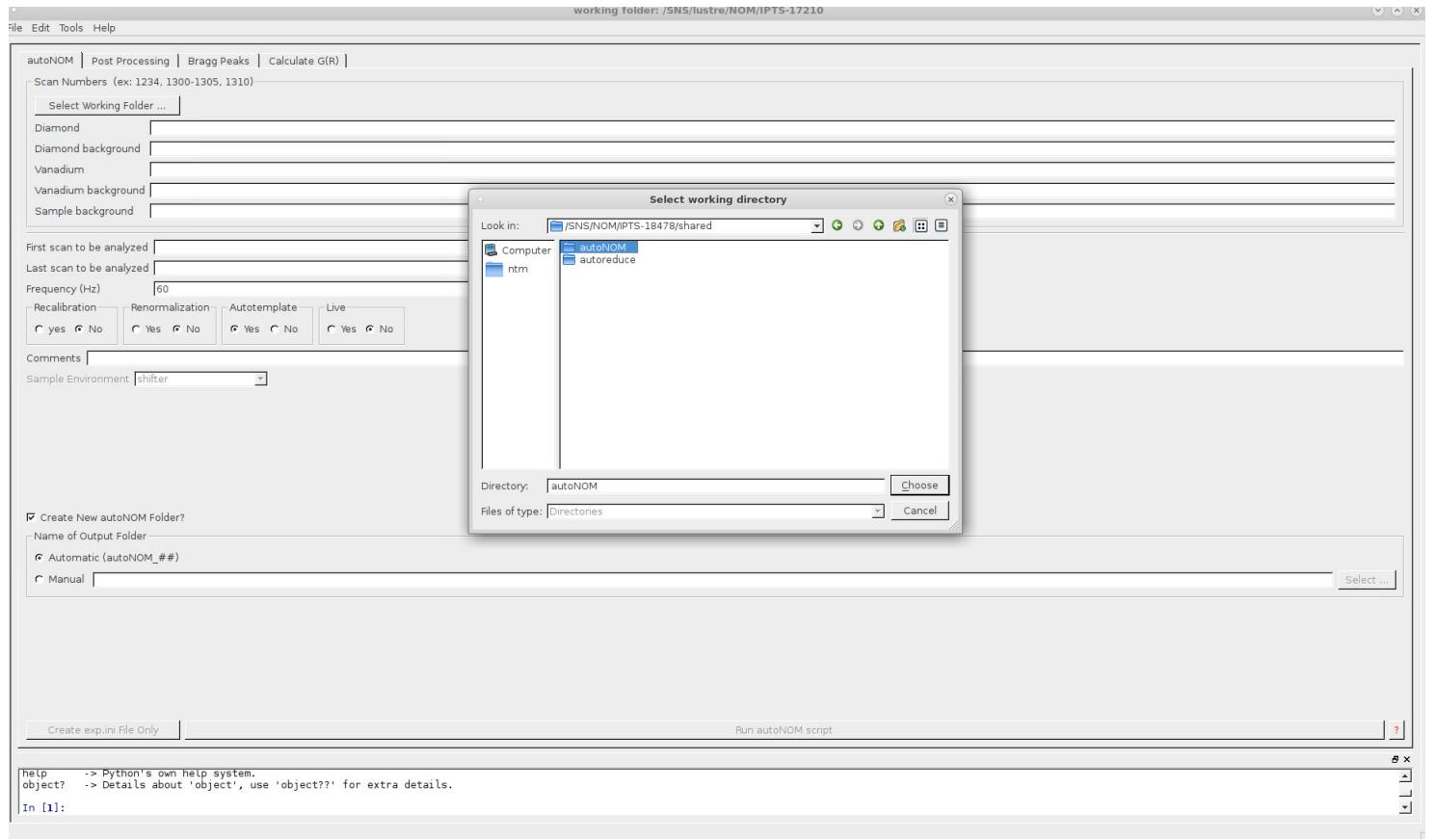
To setup the autoreduction, first launch ADDIE as described before. You will begin with the following screen with the autoreduction tab open:



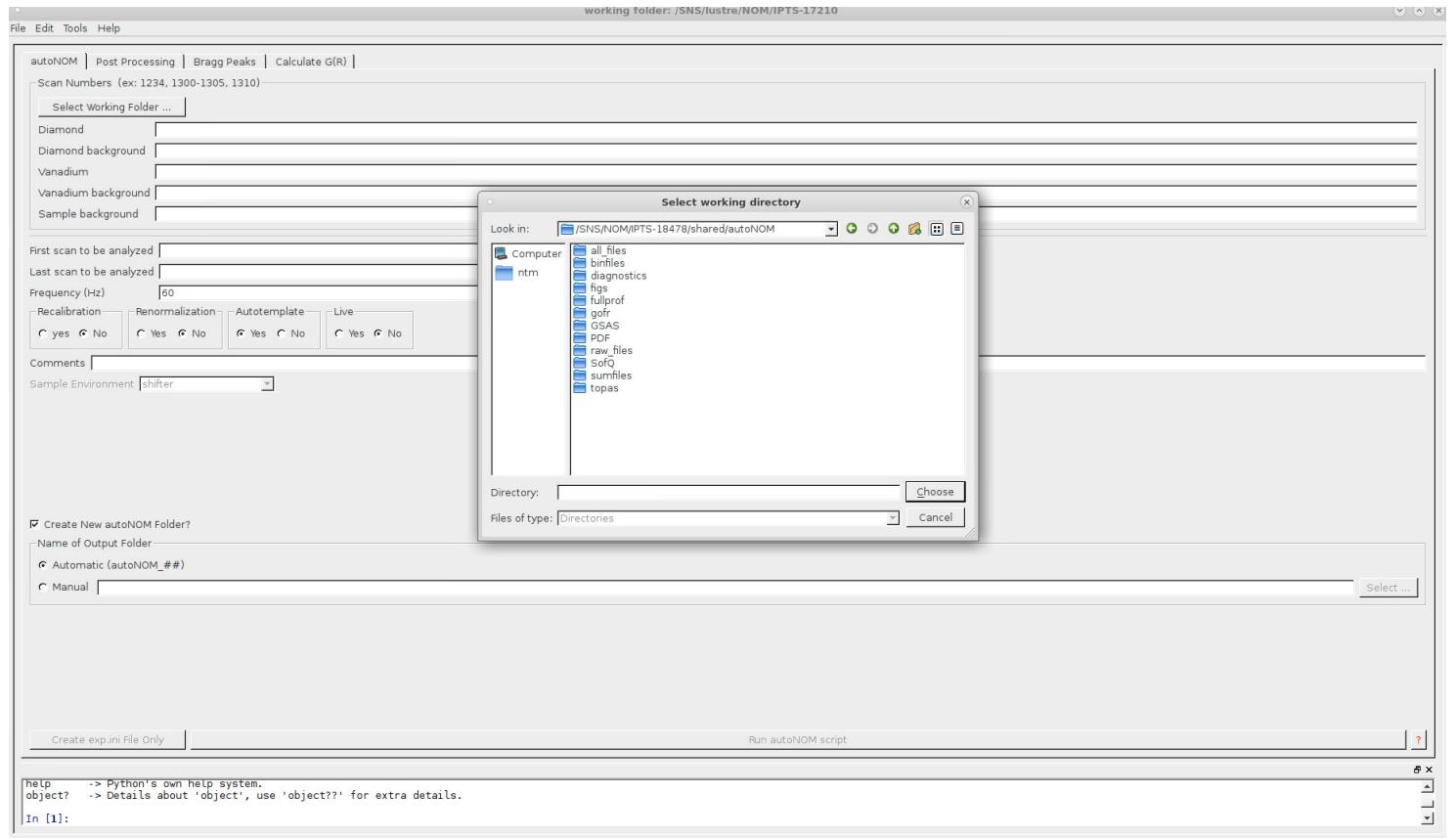
Here, we input the run numbers for the necessary measurements specified in Equation 2.1 in order to create our reduced data, Equation 2.2. To read in this data from an experiment input file (the `exp.ini` file), click on the **Select Working Folder...** button at the top. You will be presented with a 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:



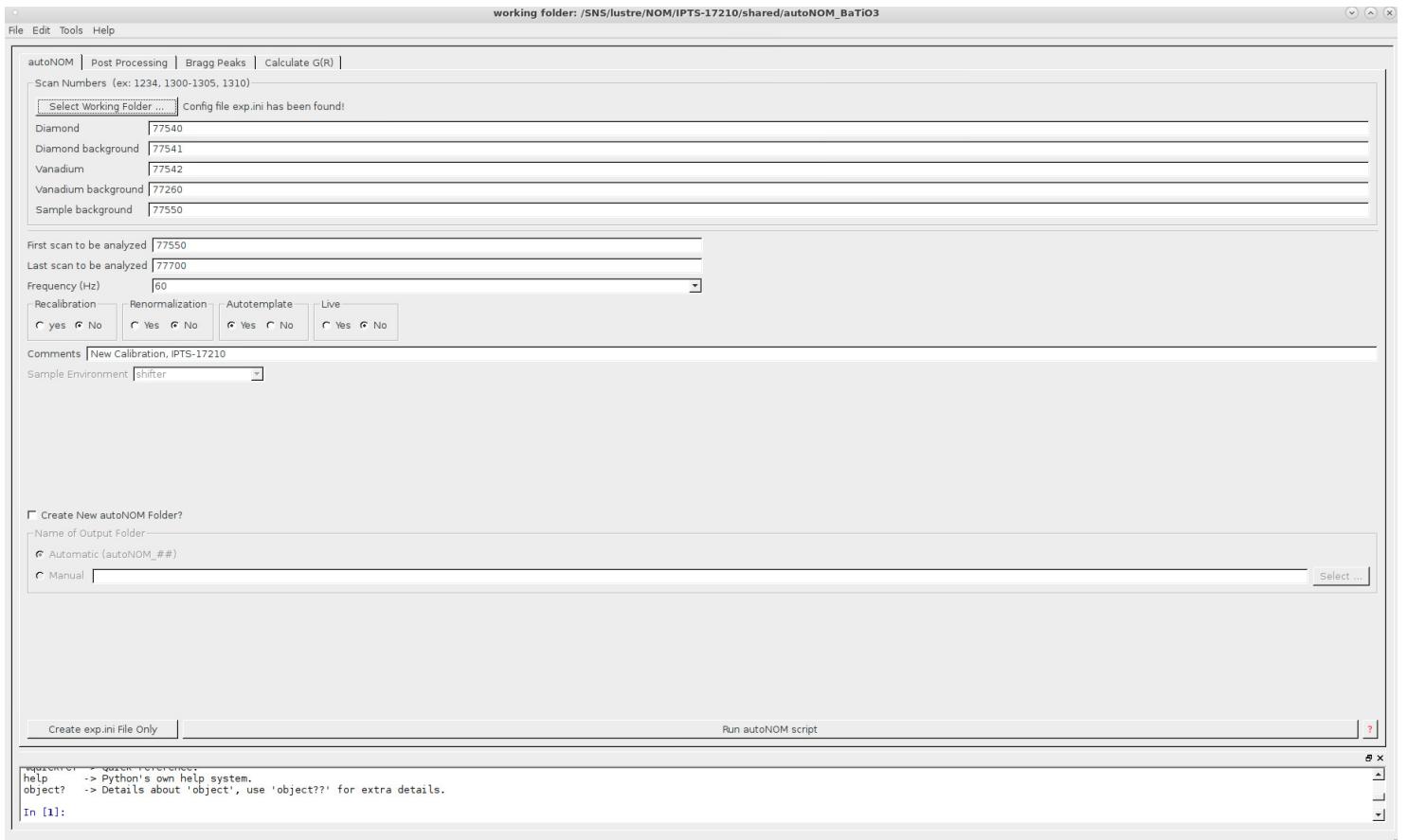
This is the file directory structure of your IPTS. You can see the `nexus` directory where the raw neutron event files are stored, the `adara` directory (ADARA = Accelerating Data Acquisition, Reduction, and Analysis) for automated live reduction files, and the `shared` directory, which is a User workspace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



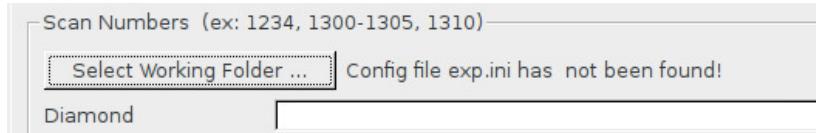
Here, the **autoNOM** directory is where we will kick off the autoreduction of AD-DIE. This will produce the **autoreduce** directory that you see above. This IPTS has already had the data reduction performed. If your IPTS has not yet had the data reduced, you may not see either of these directories. 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:

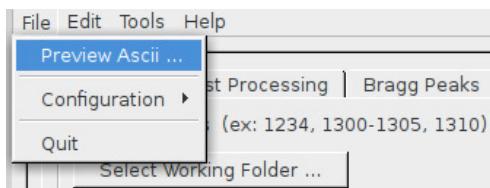
```
required ****
Dia 77540
DiaBg 77541
Vana 77542
VanaBg 77260
MTc 77550
optional ****
recali no
renorm no
autotemp yes
scan1 77550
scanl 77700
Hz 60
# New Calibration, IPTS-17210
```

### 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
```

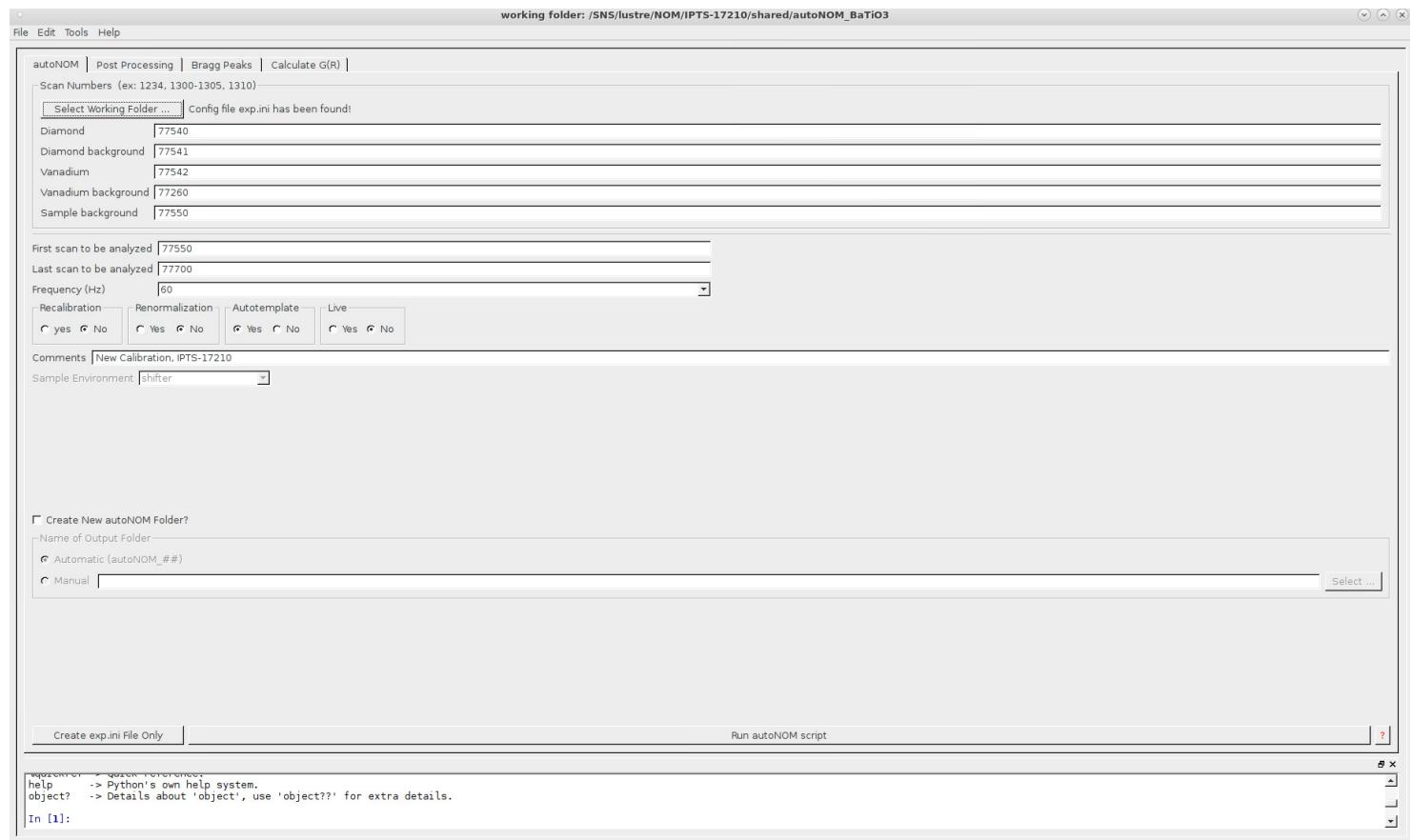
You can open this file (`los.txt` from ADDIE by going to the *File* drop-down from the *Menu* bar and selecting the *Preview Ascii...* and selecting the `los.txt` file. You can optionally use a text editor (`gedit`, `vim`, `emacs`) from a terminal.



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.

#### 4.1.3 Setting up Data Reduction

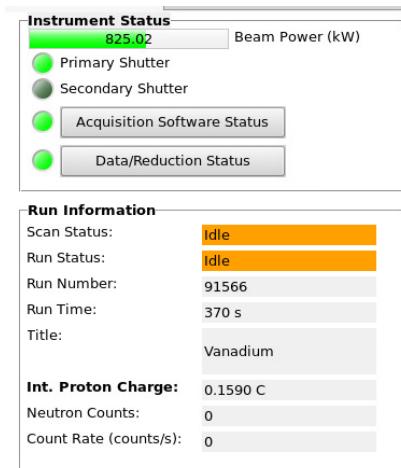
At this point, you should have experiment information input into the tab similar to the following:



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-

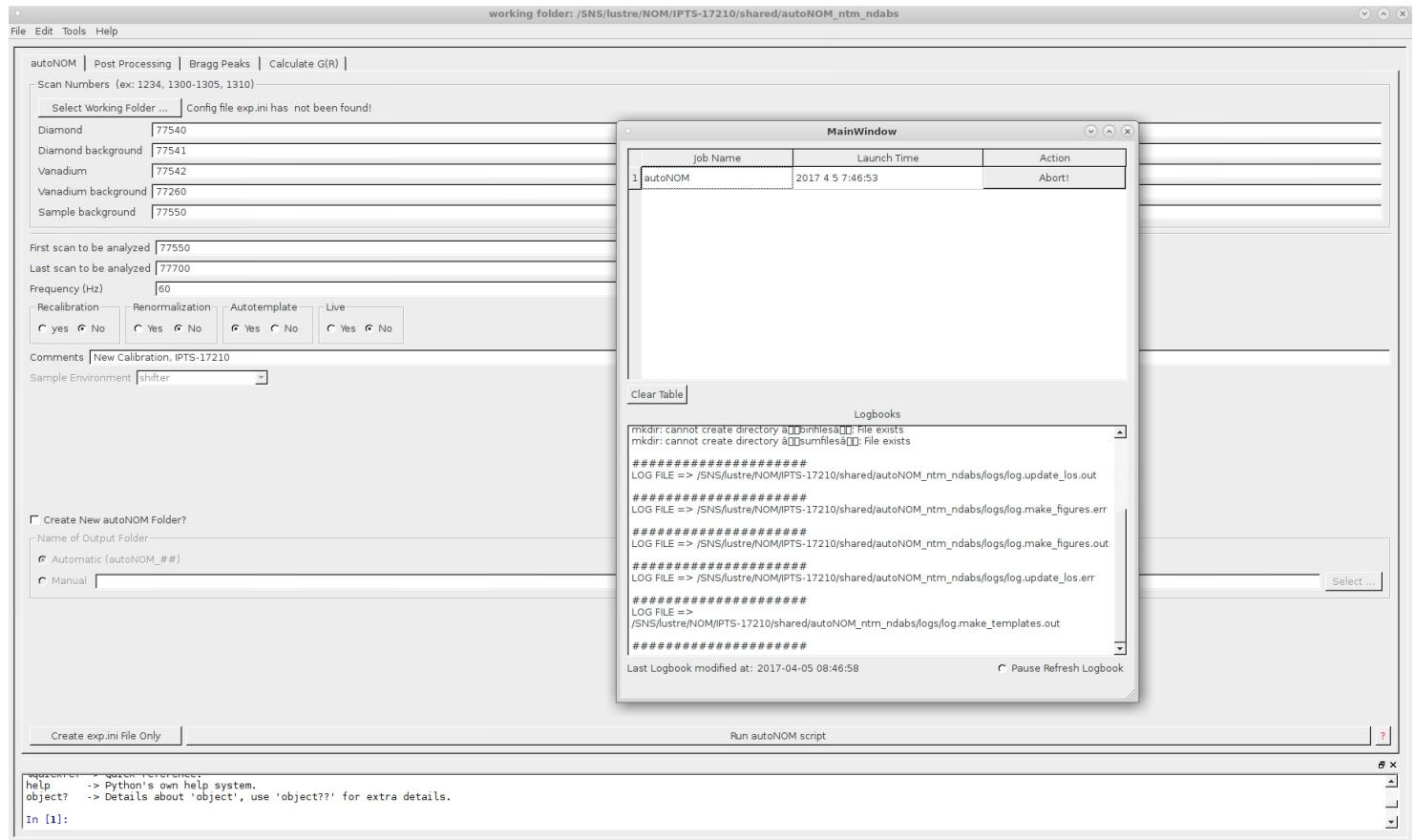
perform calibration using the input Diamond run. If the re-calibration is set to No but no calibration files are found, it will automatically perform the calibration again.

- ***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.

#### 4.1.4 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:

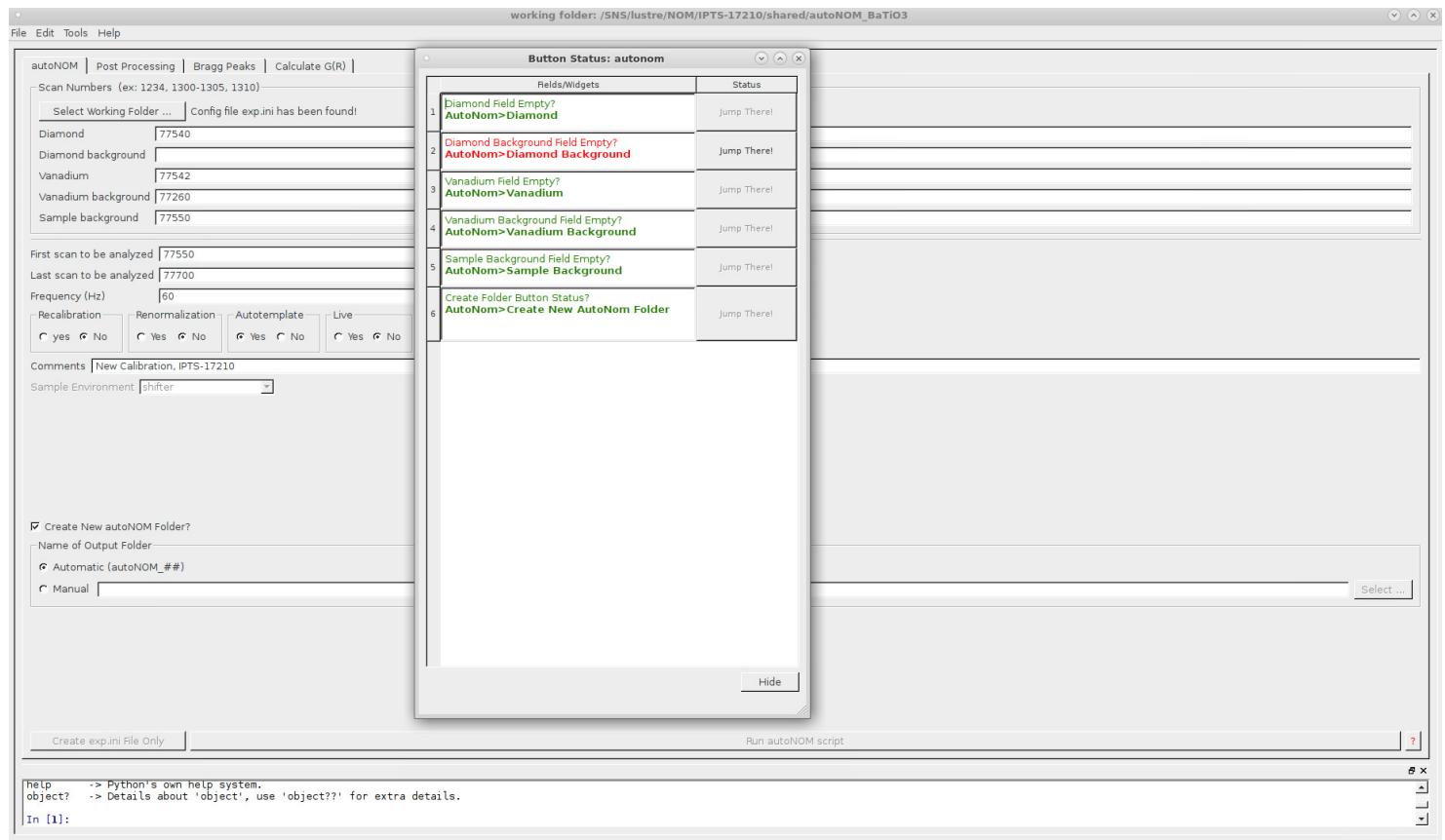


If not running in "Live" mode, you will see a display of ***Done!*** when the job is complete.

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:



#### 4.1.5 The directory structure

When the data reduction is begun (and if the autotemplate options was chosen), the `autoNOM` directory will have the following directories with the described datasets:

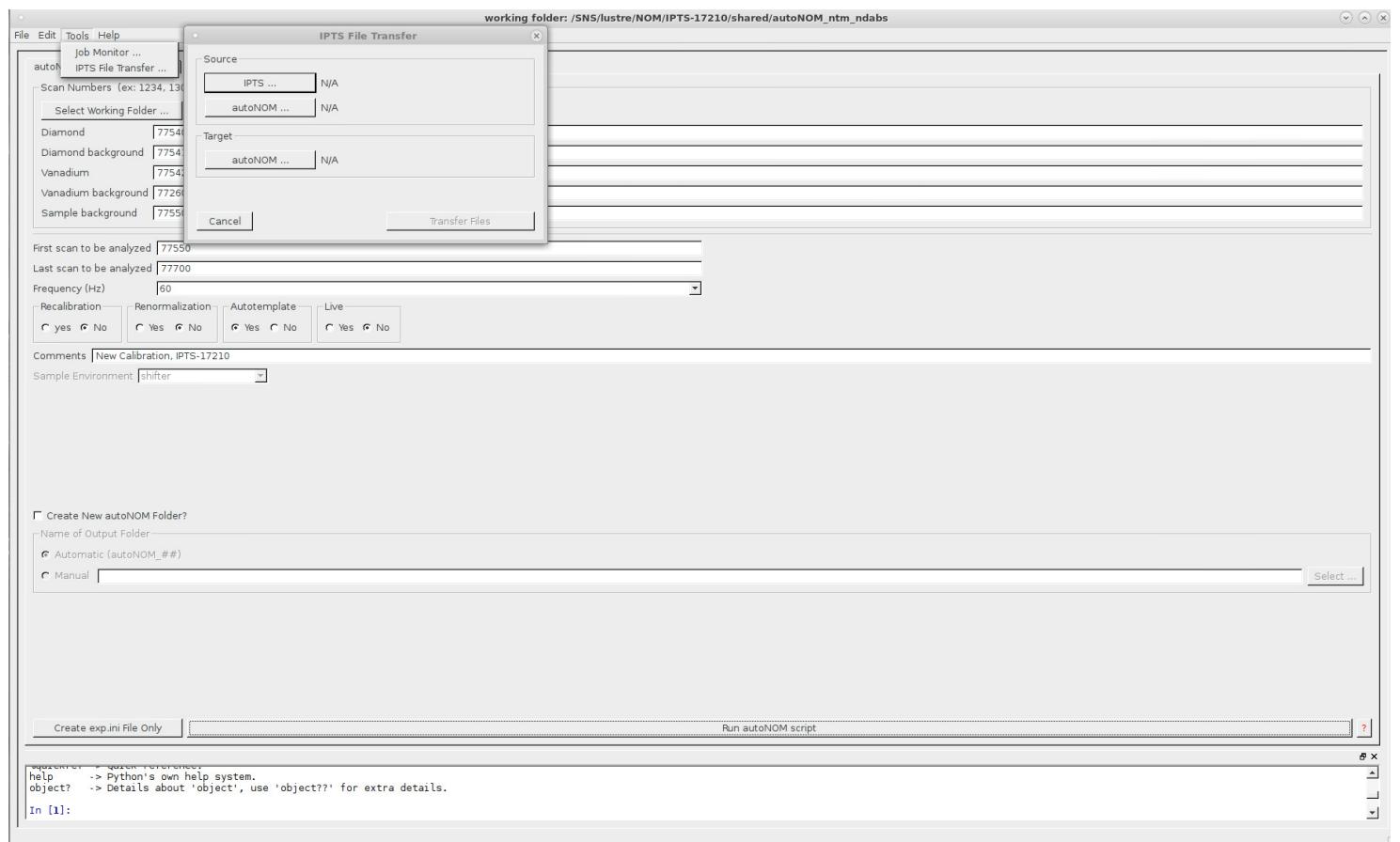
Directory	Contents
all_files	The generated IDL readable data files for individual scan number. Users will not typically interact with “all” files.
binfiles	The IDL processing finle for generating Bragg and PDF data from “all” files. Users will not typically interact with binfiles.
diagnostics	Diagnostics for the calibration performed. Plots of various data quality metrics are provided.
figs	A ”scratch” place for the User to place various saved figures.
gofr	Contains small g(r), utilized by liquids and glass community.
GSAS	Contains diffraction patterns in GSAS (*.gsa)) and PDFgetN (*.getN) readable formats for the 6 default detector arrays of NOMAD.
fullprof	Contains diffraction patterns in Fullprof (*.dat) readable format for the 6 default detector arrays of NOMAD.
logs	Logbook files for each process launched. Mainly used for debugging. Users will not typically interact with Logbooks.
PDF	Contains G(r) or PDF of your samples, in PDFgui format (*.gr)
rietveld	Contains diffraction patterns in TOPAS (*.xye) and Fullprof (*.dat) readable formats for the 6 default detector arrays of NOMAD. Produced by Mantid instead of autoNOM if launched from <b>Rietveld</b> sub-tab in <b>Post-Processing</b> tab.
SofQ	ASCII file of S(Q)-1
sumfiles	A ”scratch” directory for the User to place summed files
topas	Contains diffraction patterns in TOPAS (*.xye) readable format for the 6 default detector arrays of NOMAD.

#### 4.1.6 Getting files from another IPTS

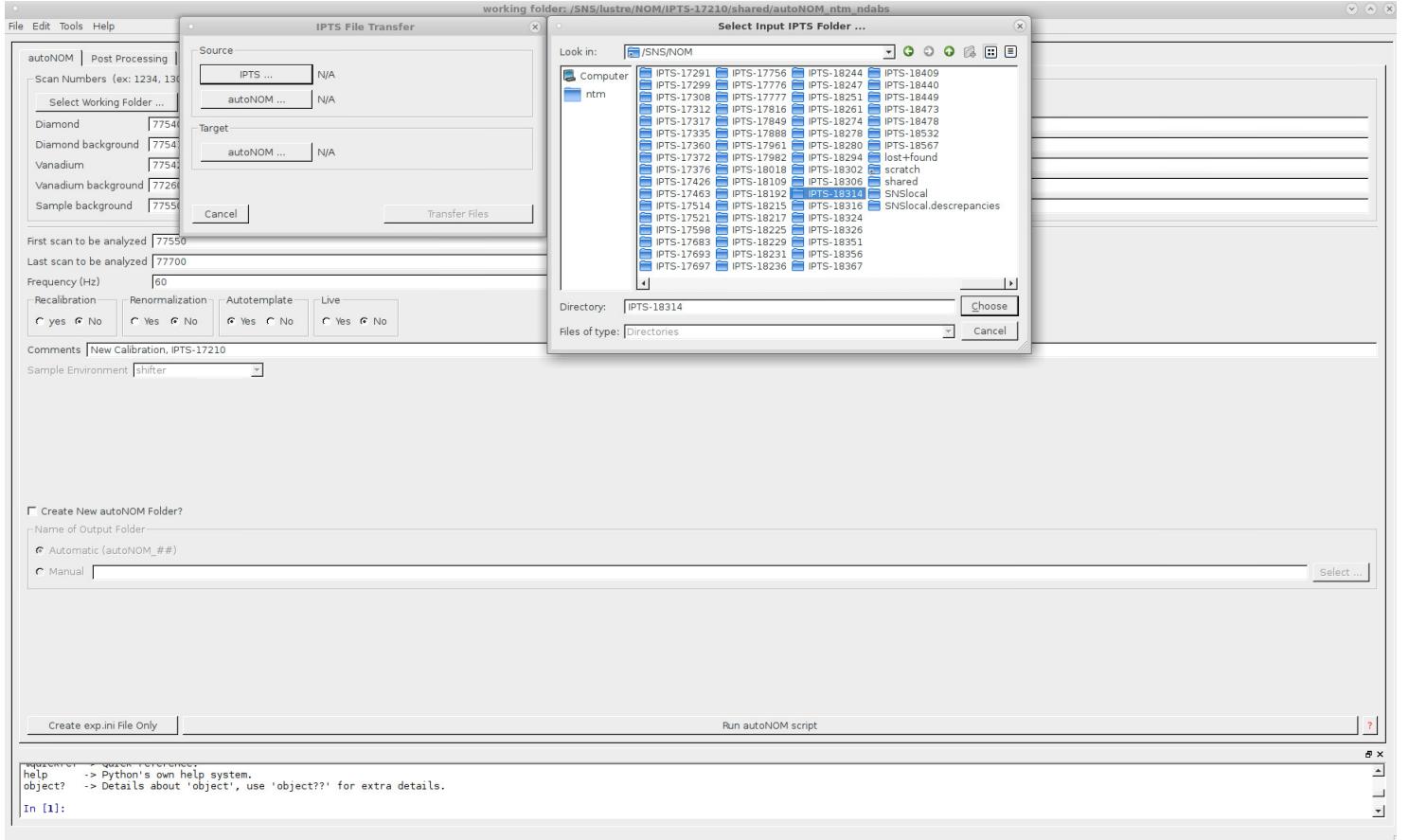
If the diamond, vanadium, and background runs where processed in another, you can use the IPTS File Transfer tool to move over those files and bypass the need to repeat the calibration and normalization steps. **NOTE:** On the **Analysis** machine, you must have the necessary permissions to access another IPTS. This may need to be performed by an Instrument Scientist with the

correct permissions. If the runs exists 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.

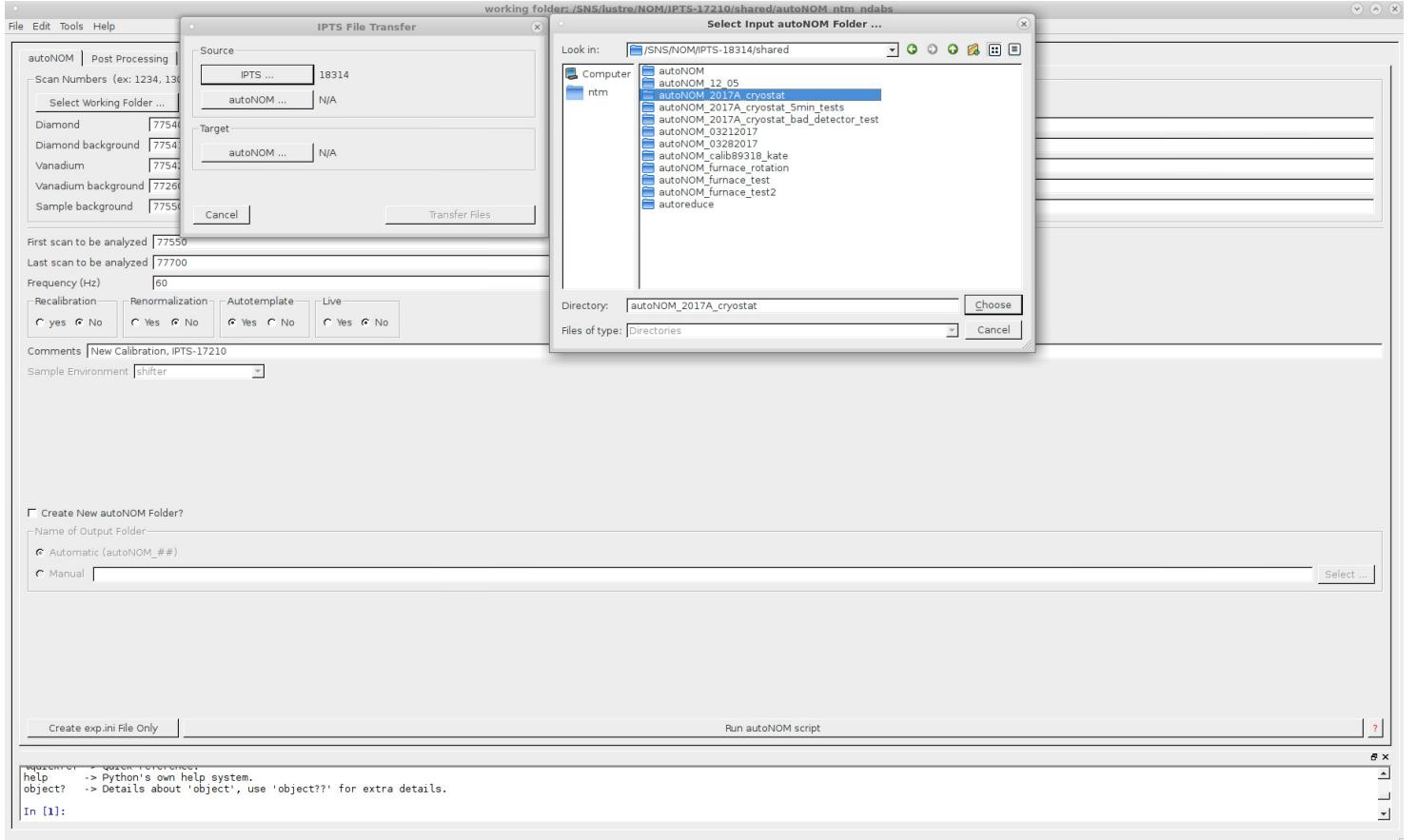
To transfer files from another IPTS, go to the **Tools** drop-down of the **Menu** bar and select **IPTS File Transfer...**. You will be presented with the following dialog box:



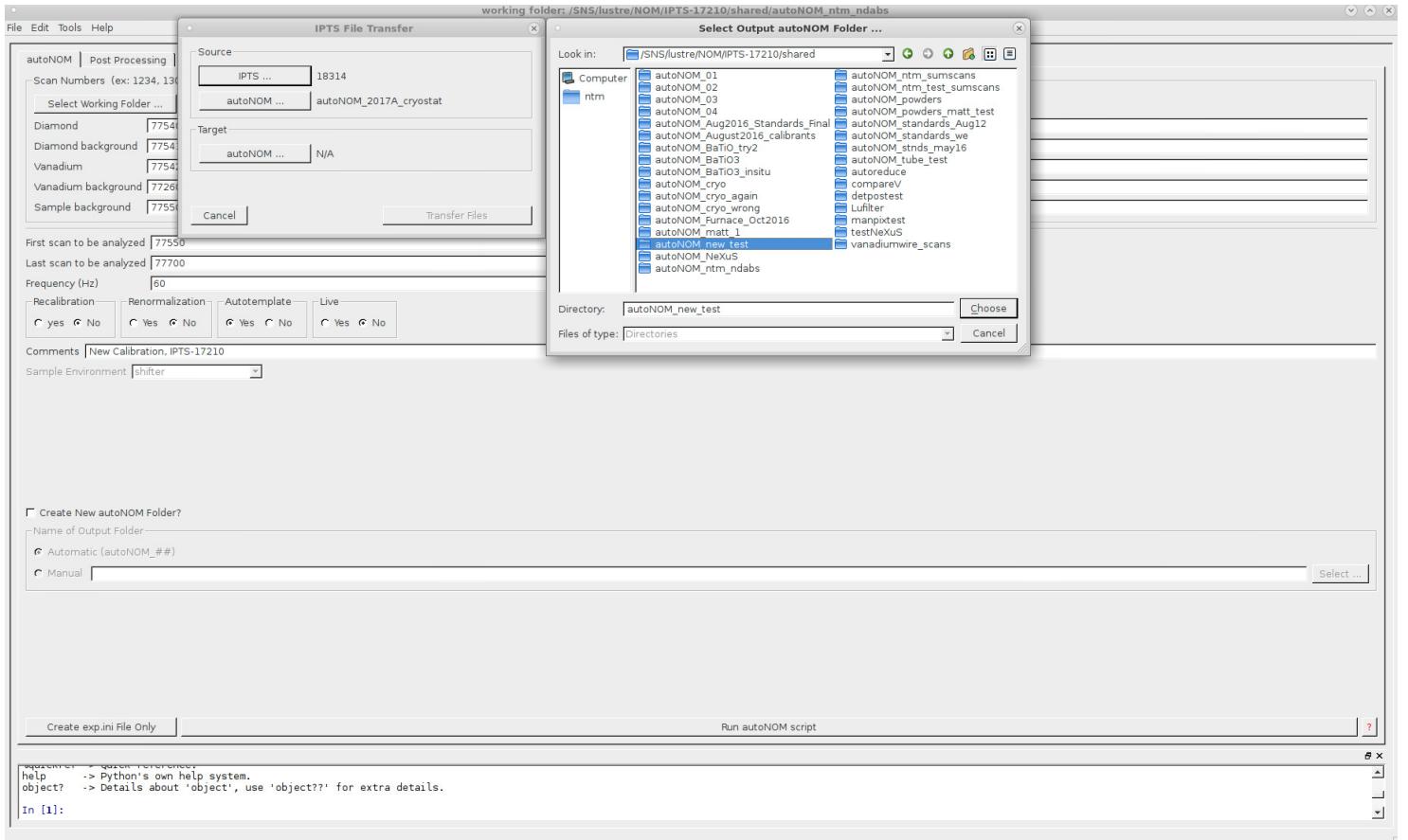
First, press the **IPTS...** button to select the IPTS from the pop-up box. Here we are selecting IPTS-18314. Press **Choose** once selected::



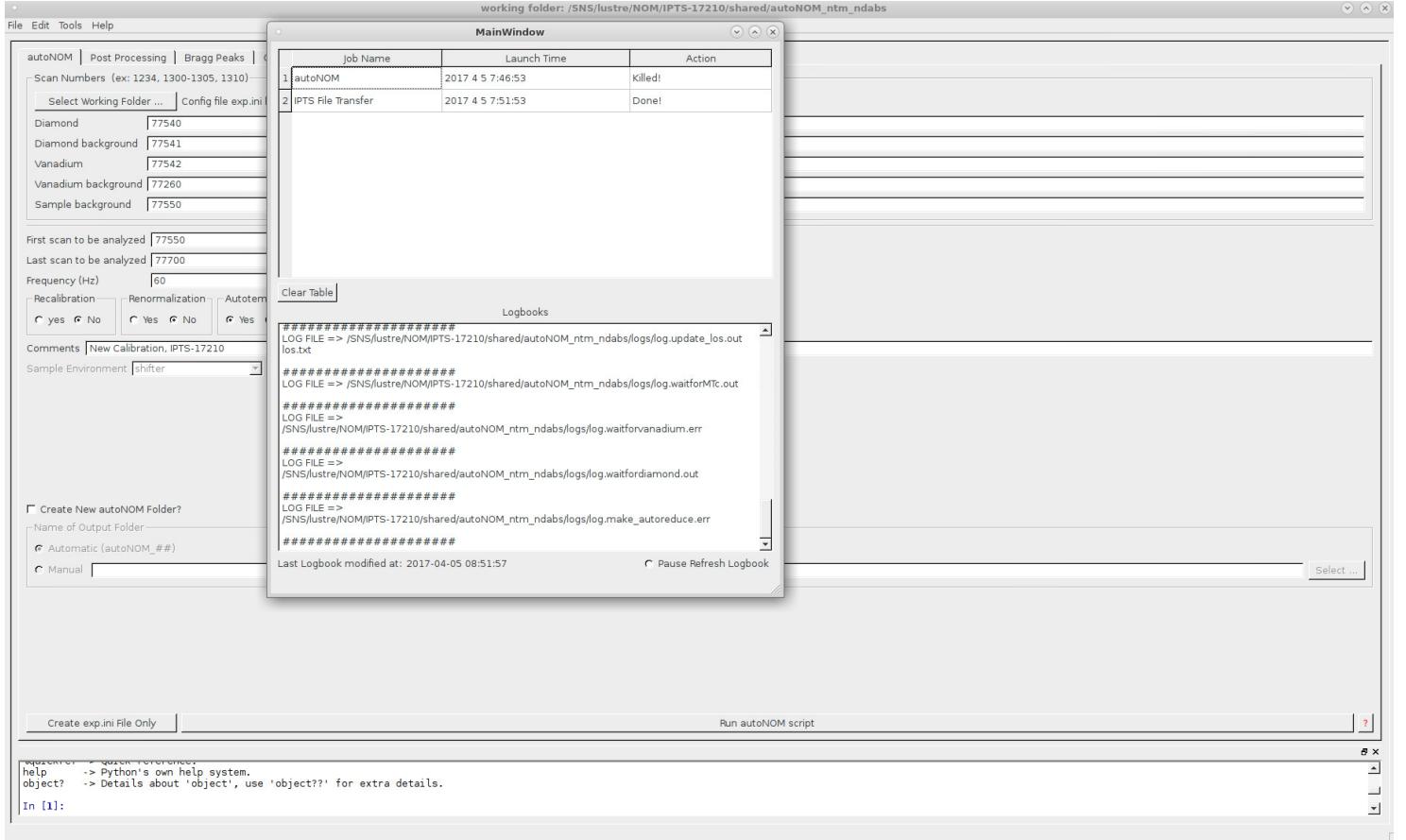
Then, press the ***autoNOM...*** button in the **Source** section to select the specific autoNOM directory. From below, you can see that an IPTS can have multiple autoNOM directories. We are selecting the autoNOM\_2017A\_cryostat below. Press ***Choose*** once selected:



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.

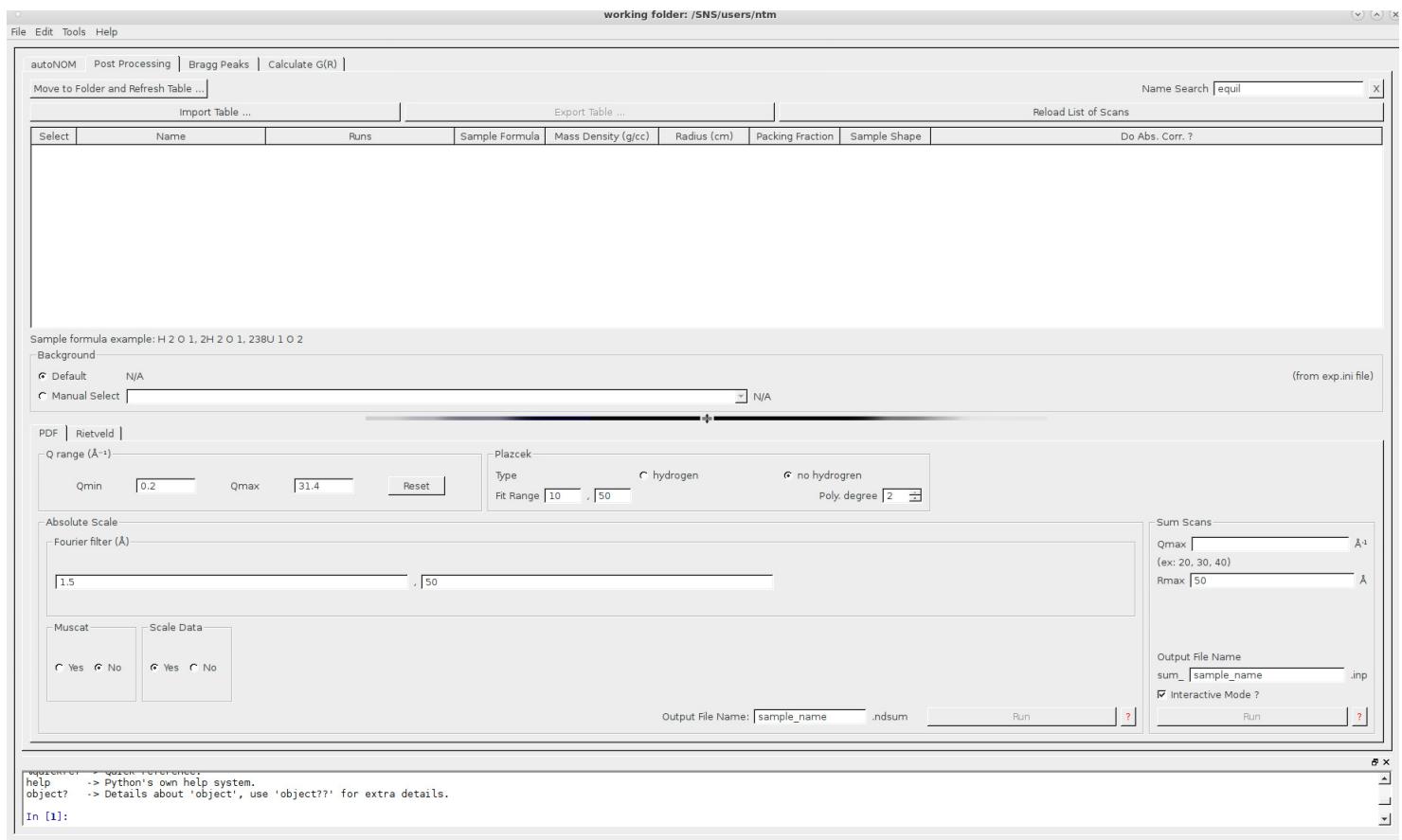


## 4.2 Post-Processing of runs

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.

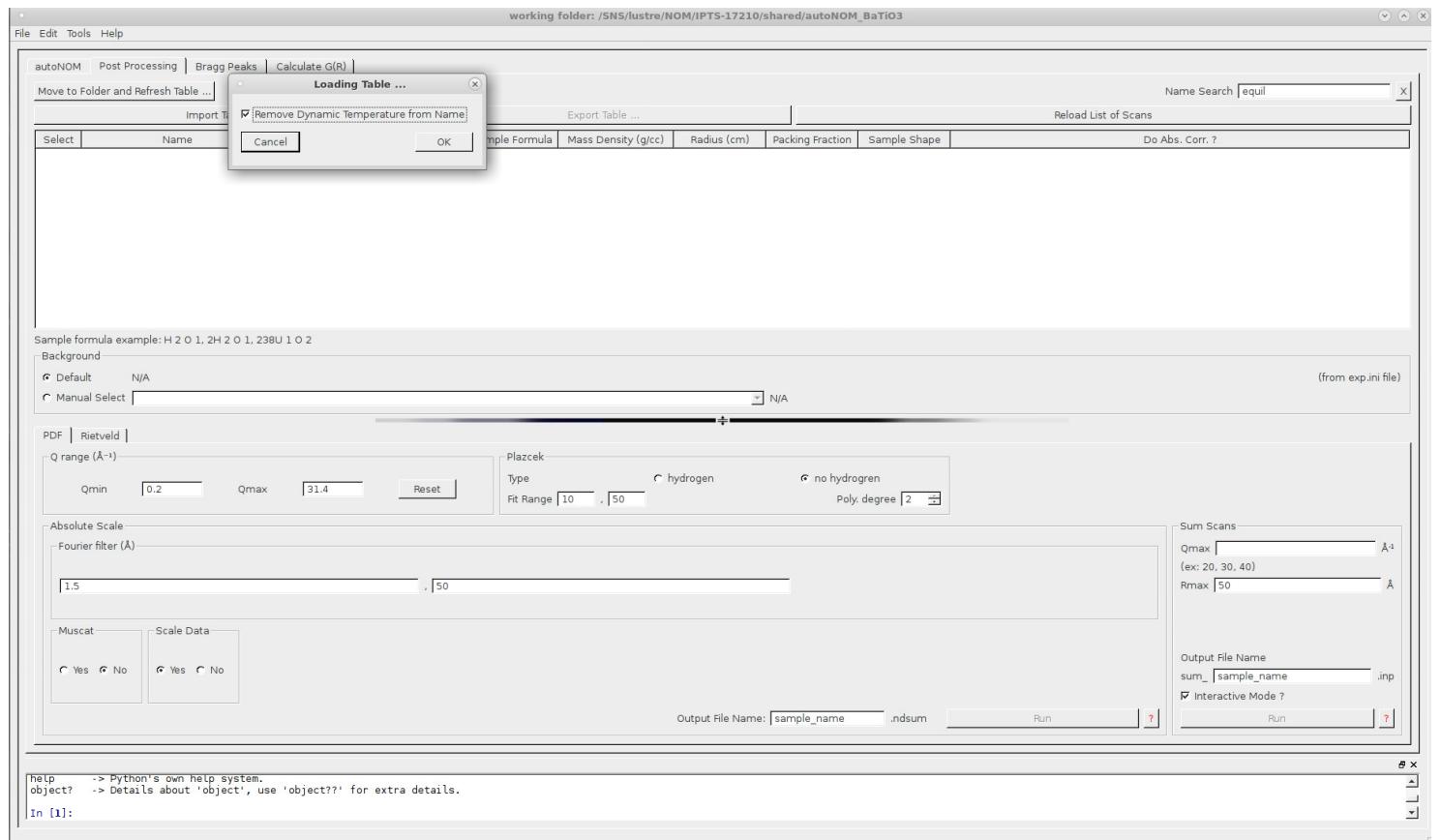
### 4.2.1 Load Runs into Table

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

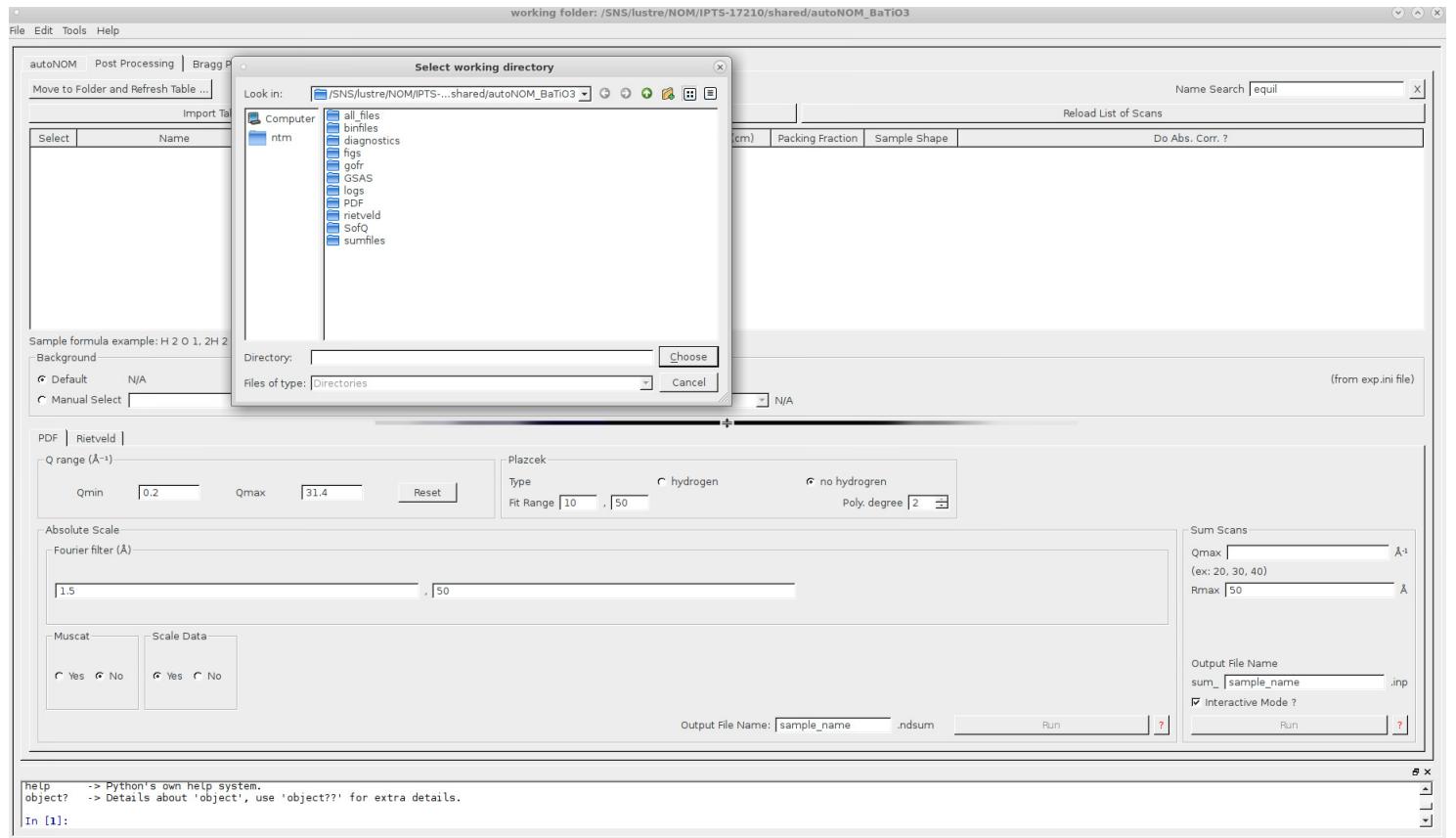


From here, we must first import our individual run information into the table. We do so by selecting the ***Move To Folder and Refresh Table...*** button. We are presented with the following dialog box asking about the Dynamic Temperature. From the individual runs, the actual temperature of the experiment 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 BaTiO<sub>3</sub>. 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 BaTiO<sub>3</sub>, BaTiO<sub>3</sub>\_350K, MT\_3p5\_for\_44CaSiO<sub>3</sub>, 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 for BaTiO<sub>3</sub> is shown with its sample formula: 77551,77552,77553,77554,77555,77556,77557,77558,77559,77560,77561,77562,77563,77564,77565,77566,77567,77568,77569,77570,77571,77572,77573,77574,77575,77576,77577,77578,77579,77580,77581,77582.

The interface includes sections for PDF/Rietveld analysis, Q range (Å<sup>-1</sup>), Plazek parameters (Type: hydrogen, Fit Range: 10 to 50, Poly. degree: 2), Absolute Scale (Fourier filter: 1.5 to 50 Å), and Sum Scans (Qmax: 20, 30, 40 Å<sup>3</sup>, Rmax: 50 Å). There are also Muscat and Scale Data options, and an Output File Name field (sum\_ [sample\_name].inp) with an Interactive Mode checkbox.

A command-line interface at the bottom shows help and object information:

```
help      -> Python's own help system.
object?  -> Details about 'object', use 'object??' for extra details.
In [1]:
```

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:



#### 4.2.2 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.

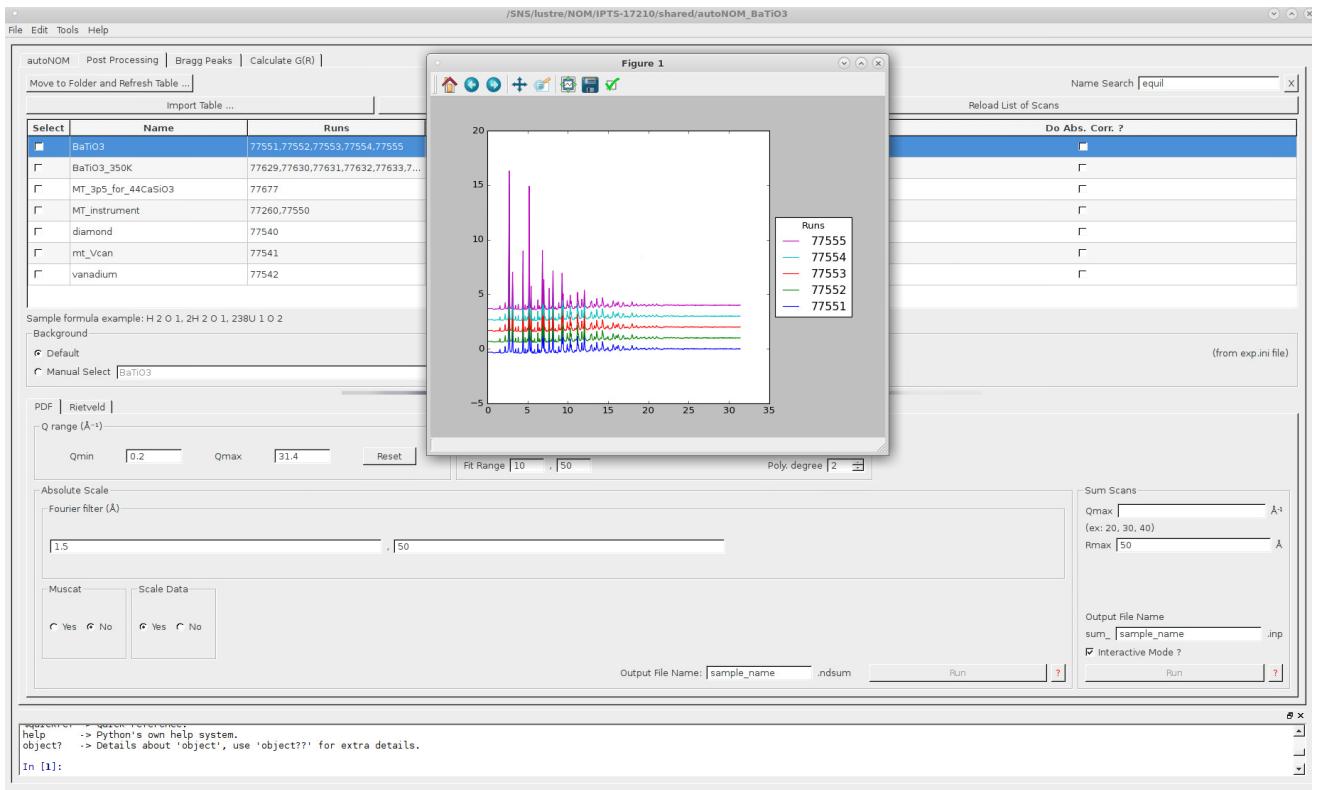
To edit any of the fields in the table, you can just double click and input any information you would like. This includes changing the name of the group or deleting runs for a given row. You can select multiple rows by holding the *Ctrl* button for individual selections or holding down *Shift* to chose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

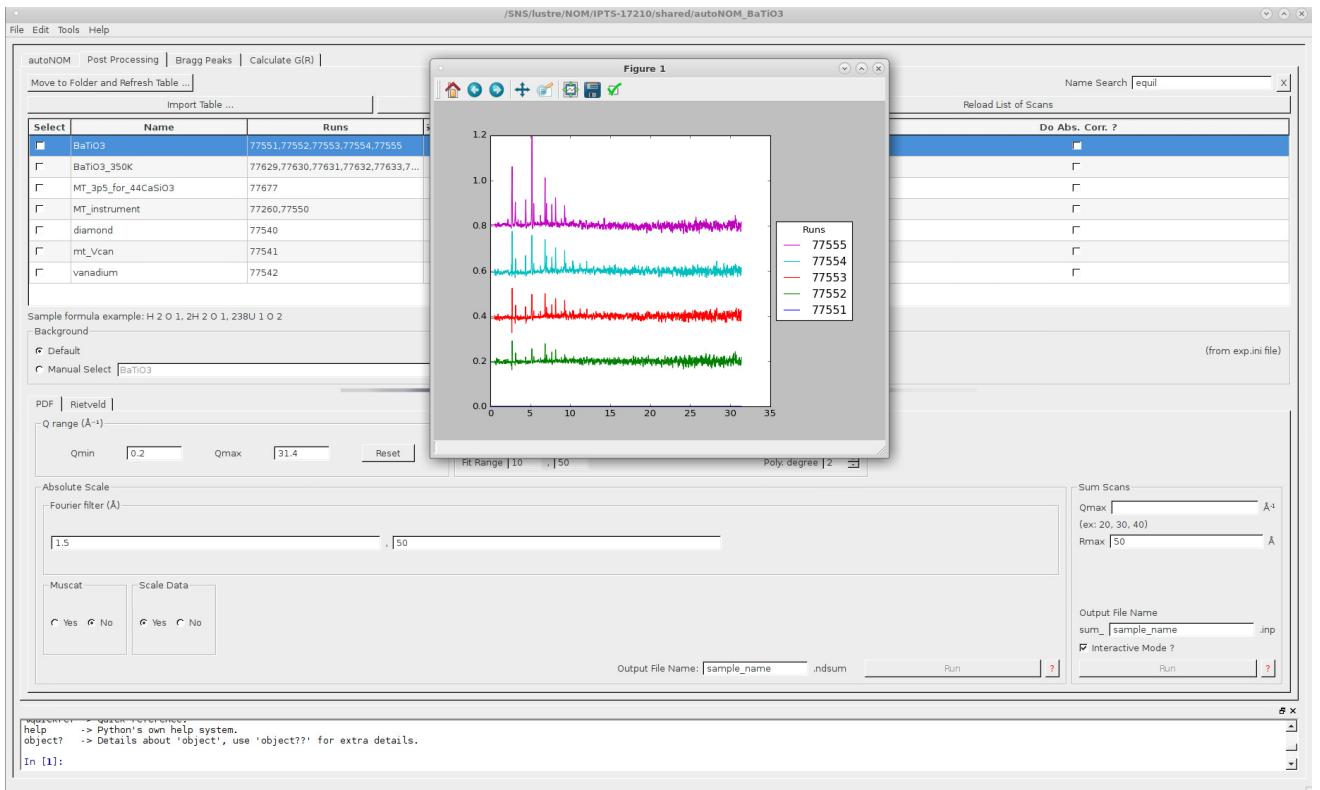
- Top Bar:** File, Edit, Tools, Help, /SNS/lustre/NOM/IPTS-17210/shared/autoNOM\_ntm\_ndabs
- Toolbar:** autoNOM, Post Processing, Bragg Peaks, Calculate G(R), Move to Folder and Refresh Table ...
- Table:** A grid of experimental runs with columns: Select, Name, Runs, sample formula, Mass Density (g/cc), Radius (cm), Packing Fraction, Sample Shape, Do Abs. Corr.?, and a Name Search field.
- 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)
- Plot Area:** Shows a plot of Intensity vs. Q-range (Å⁻¹) with a peak labeled "BaTiO3". Options include Plot, Plot Diff (1st run), Plot Diff (Avg.), Refresh/Reset Table, and Clear Table.
- Absolute Scale:** Fourier filter (Å⁻¹) with a scale bar from 1.5 to 50.
- Muscat:** Scale Data options (Yes/No).
- Sum Scans:** Sum Scans, Qmax (ex: 20, 30, 40) Å⁻¹, Rmax 50 Å, Output File Name: sample\_name.inp, Interactive Mode? (checkbox), Run, ?.
- Bottom:** Python help text and In [1]:

These options are as follows:

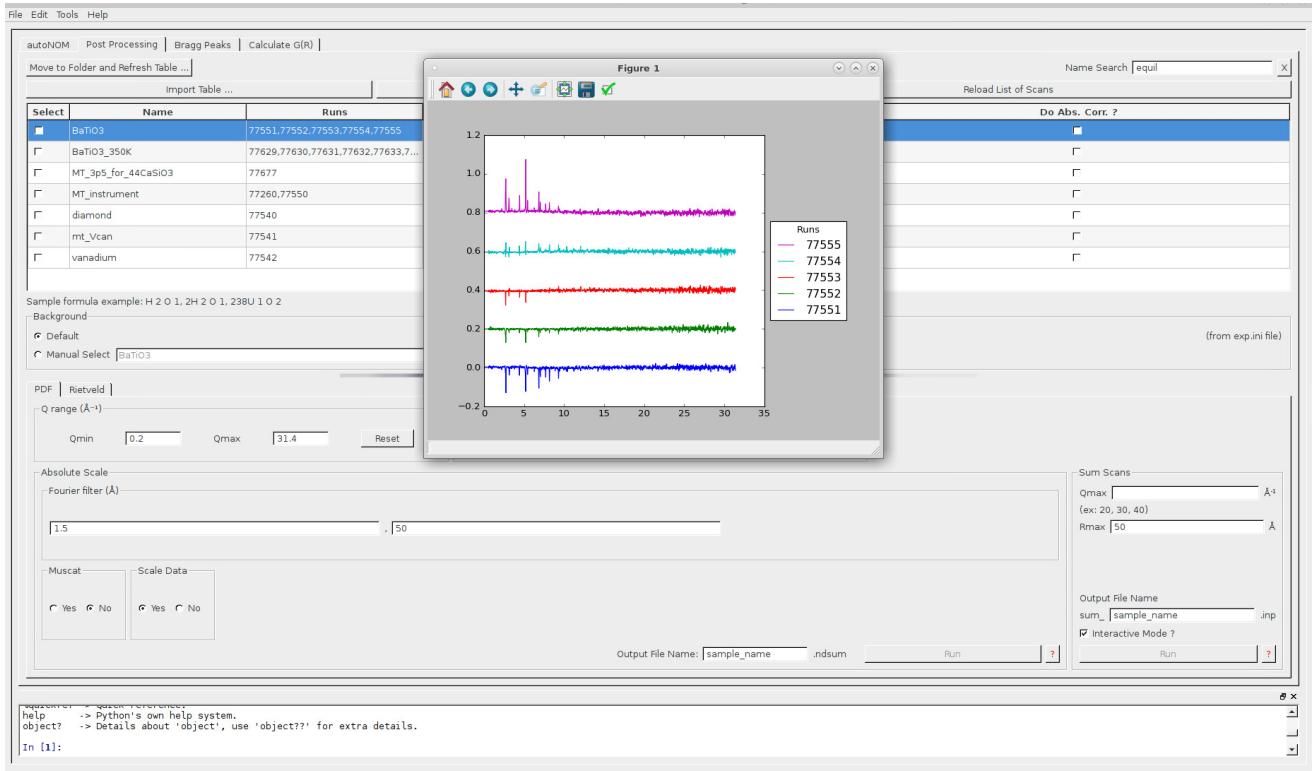
- ***Undo***: Undo the last action in the table.
- ***Redo***: Redo the last undone action in the table.
- ***Copy***: Copy the selected contents of a field in a row.
- ***Paste***: Paste copied contents in a field of a row.
- ***Clear***: Clear the contents of a field in a row.
- ***Check All***: Check 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:

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 BaTiO<sub>3</sub> and BaTiO<sub>3</sub>\_350K rows that were selected based on a match with the "BaTi" input in the **Name Search**.

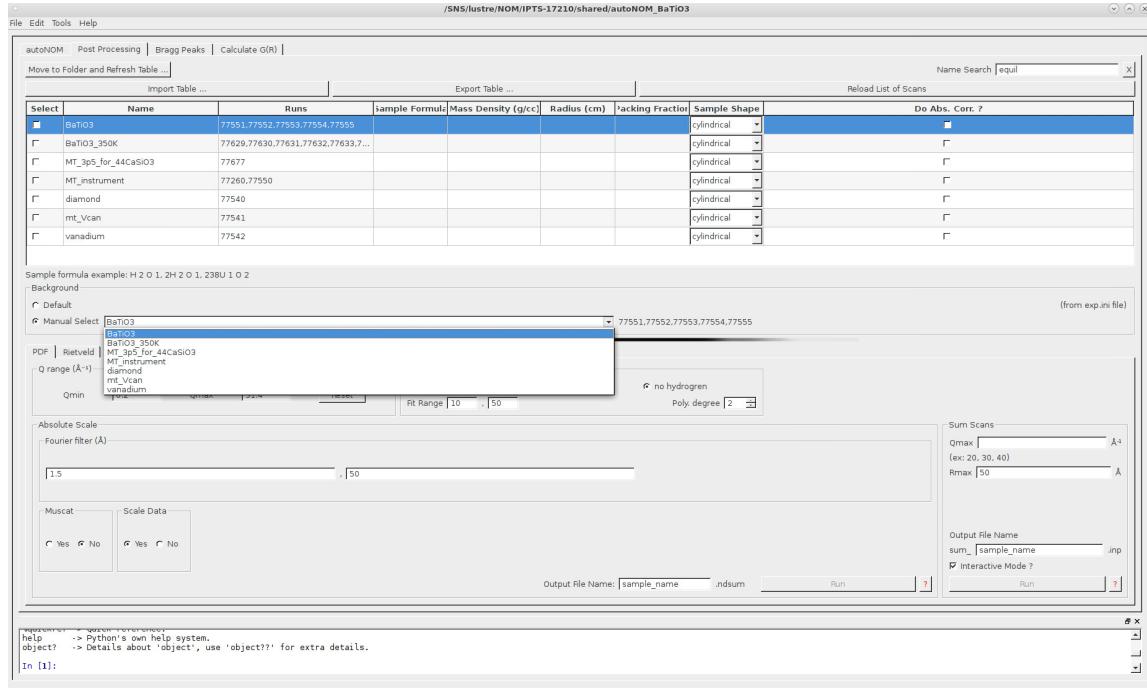
The screenshot shows a software window titled "autoNOM Post Processing | Bragg Peaks | Calculate G(R) | /SNS/lustre/NOM/IPTS-17210/shared/autoNOM\_BaTiO3". The main area is a table with the following data:

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.

#### 4.2.3 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 [SNSPowderReduction](#) script).

## 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.

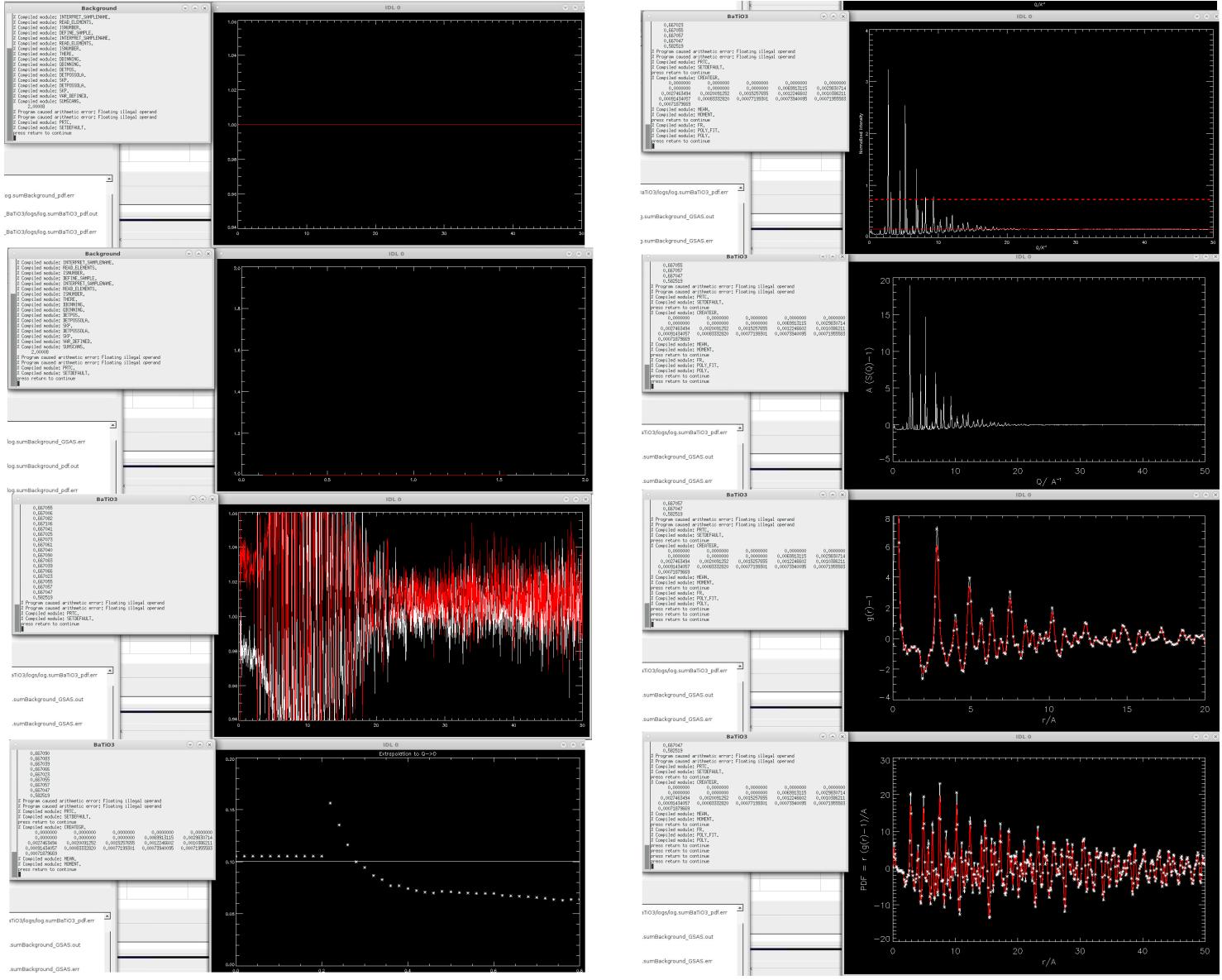
***Qmax*** allows for a list to use for the summed S(Q) datasets, where a simple truncation is performed.

***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  $Q \rightarrow \inf$  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 progresss. The **Rietveld** Tab is shown below:

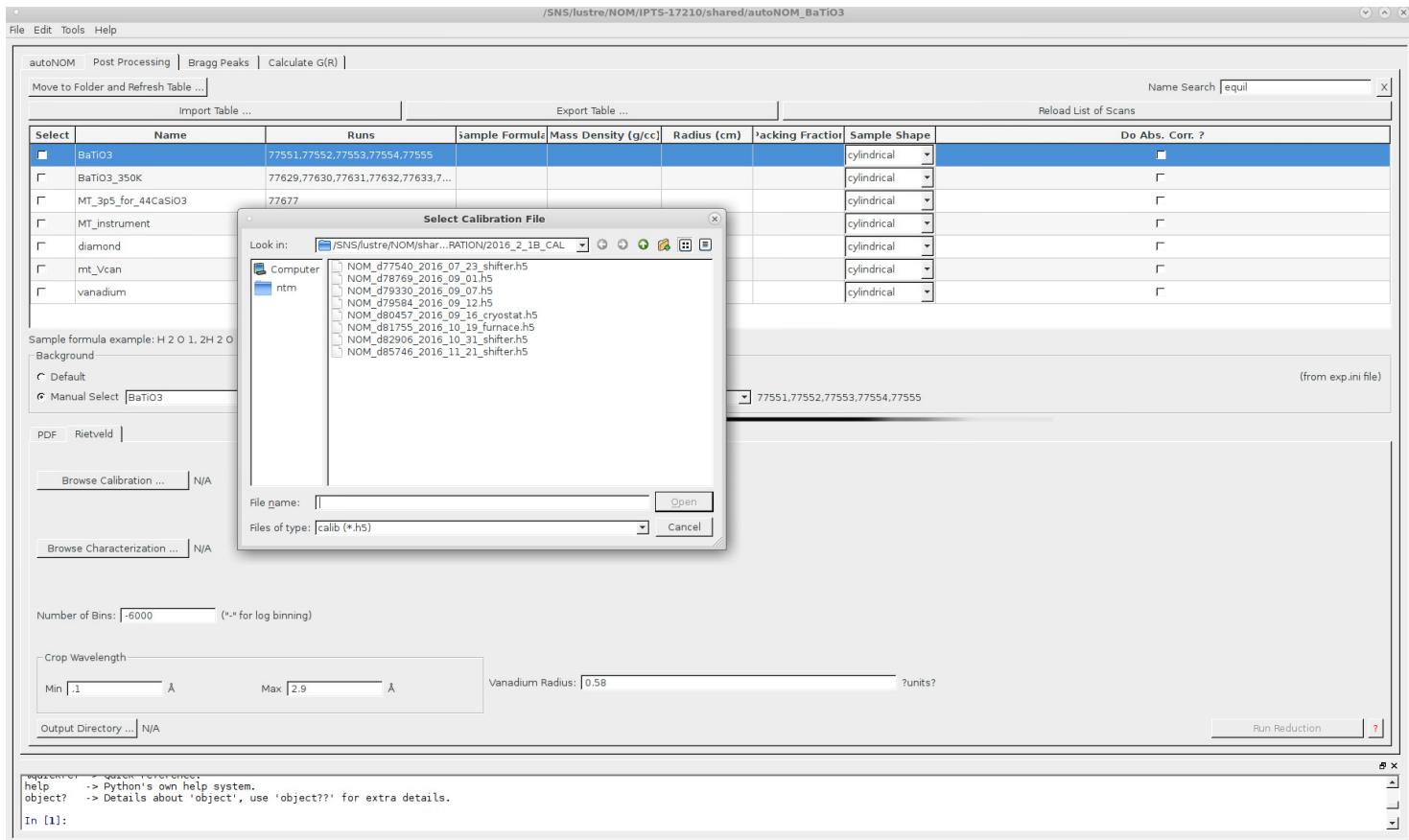
The screenshot shows the autoNOM software interface with the following details:

- 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 for BaTiO3. The columns include Select, Name, Runs, Sample Formula, Mass Density (g/cc), Radius (cm), Packing Fraction, Sample Shape, and Do Abs. Corr. ?.
 

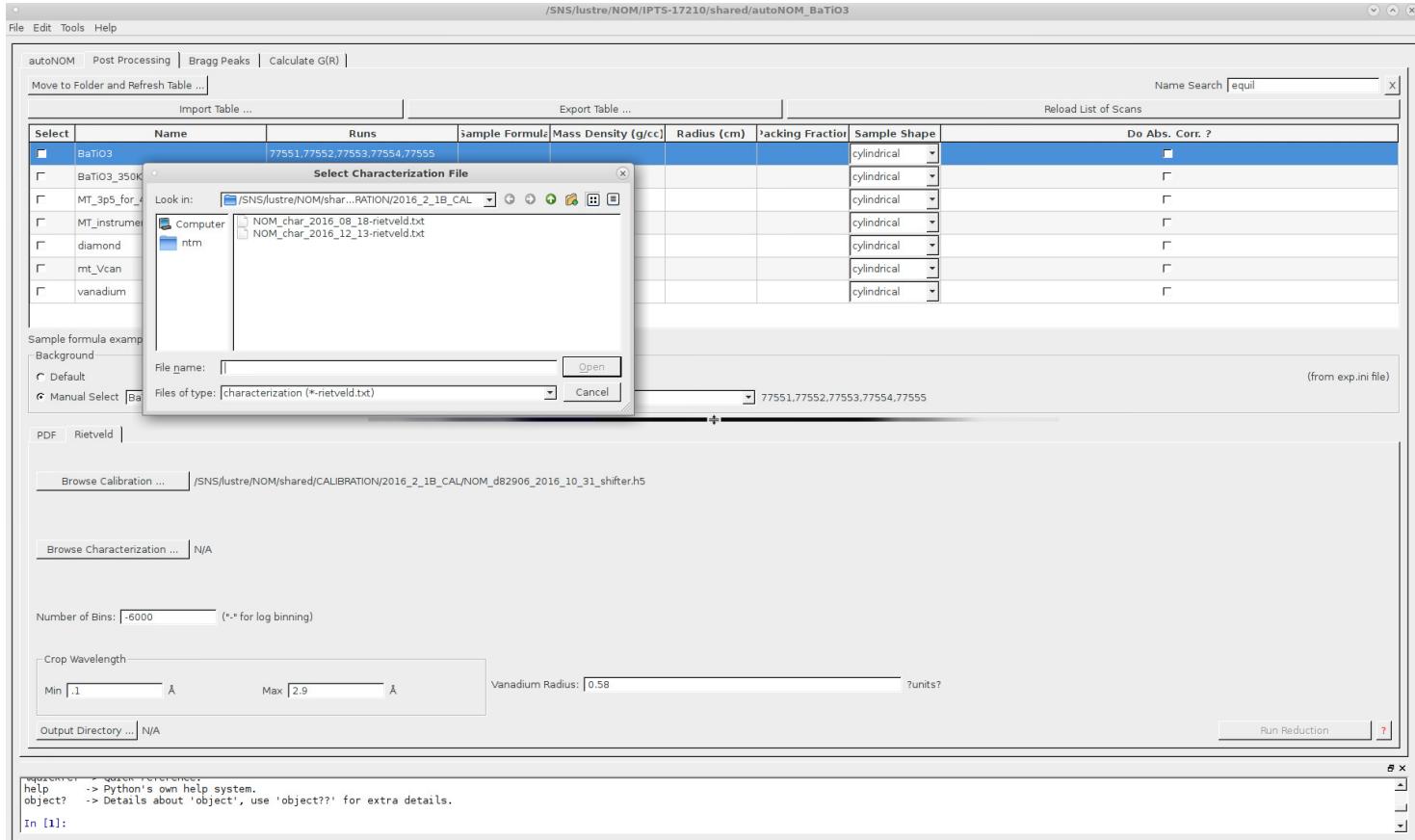
Select	Name	Runs	Sample Formula	Mass Density (g/cc)	Radius (cm)	Packing Fraction	Sample Shape	Do Abs. Corr. ?
<input checked="" type="checkbox"/>	BaTiO3	77551,77552,77553,77554,77555				cylindrical	<input checked="" type="checkbox"/>	
<input type="checkbox"/>	BaTiO3_350K	77629,77630,77631,77632,77633,7...				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"/>	
- Background Selection:** Default (radio button) or Manual Select [BaTiO3] (dropdown menu) with value 77551,77552,77553,77554,77555 (from exp.ini file).
- Processing Options:** PDF, Rietveld, Browse Calibration ..., Browse Characterization ..., Number of Bins: 6000 (N/A), Crop Wavelength (Min: .1 Å, Max: 2.9 Å), Vanadium Radius: 0.58 Å, Output Directory ... (N/A), Run Reduction, In [1]:
- Help:** Python's own help system, object? -> 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:

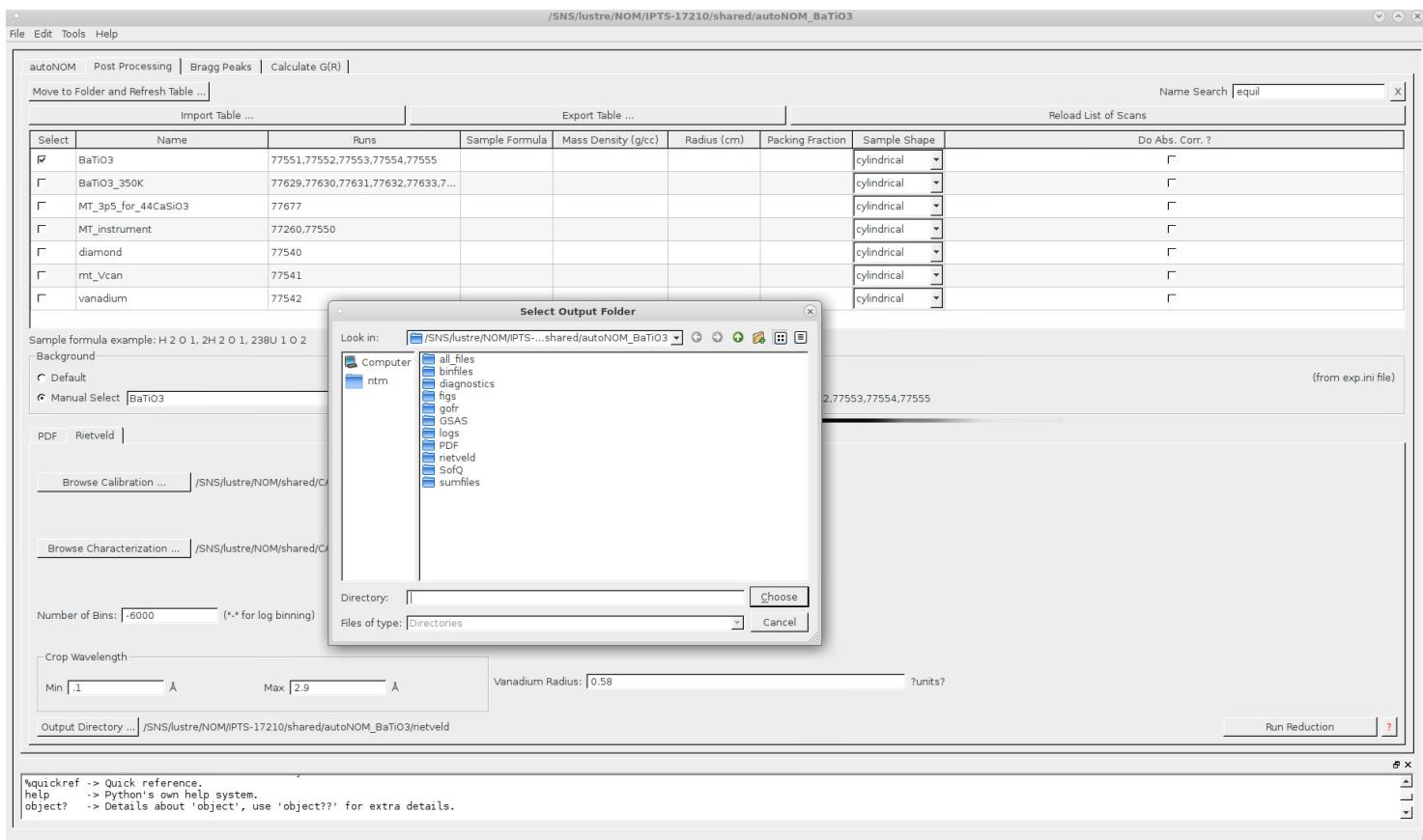


- **Browse Characterization...:** Next, you must also select a characterization file for the instrument. Press the **Browse Characterization...** button to browse the characterization files available commonly shared to all NOMAD Users. Select one that is the most recent. You will see something similar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

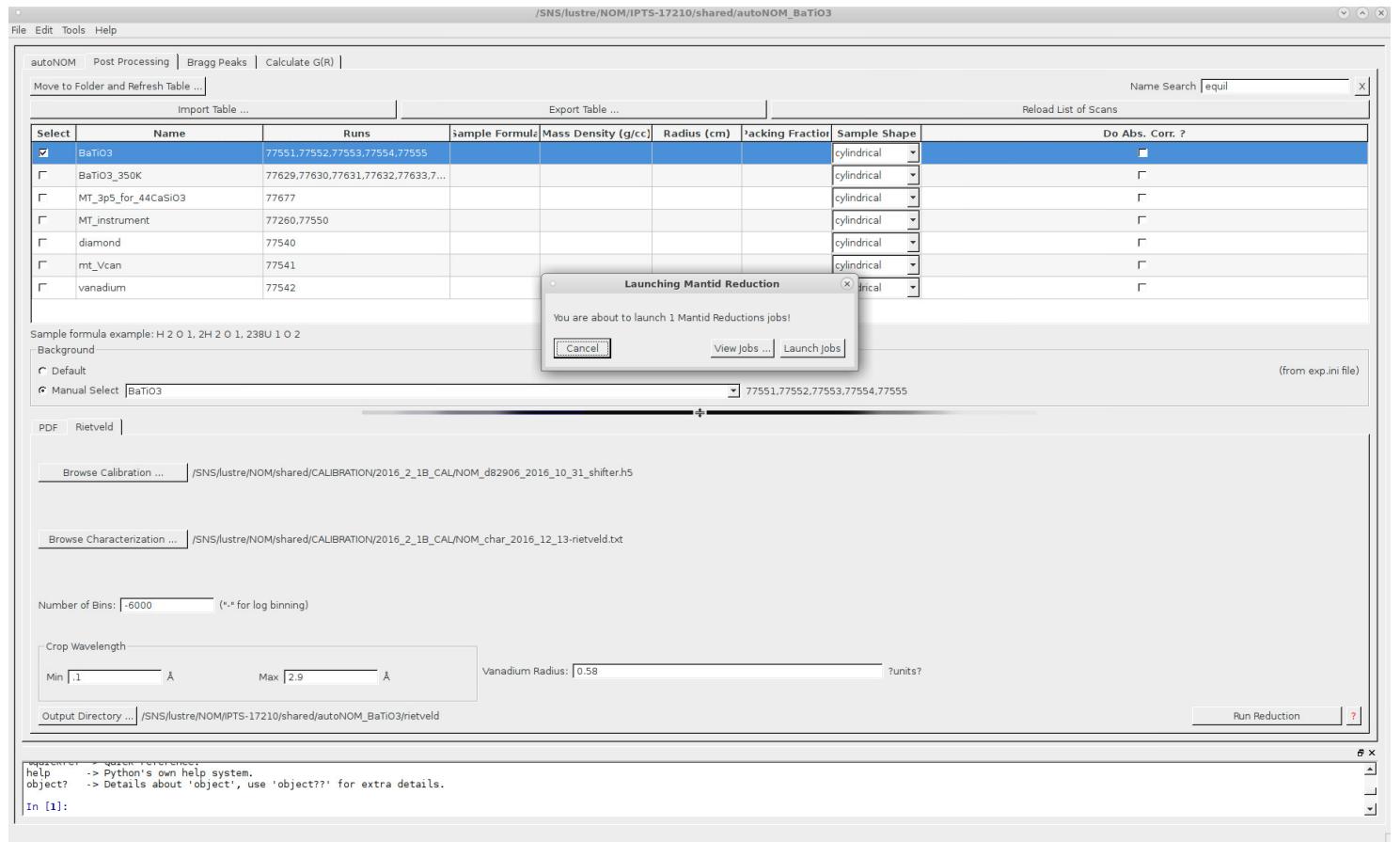


- **Number of Bins:** This defines the number of bins used along the x-axis. A negative value implies logarithmic binning, using the formula  $x_{i+1} = x_i(1 + |\Delta x_i|)$ . More detail can be found [here](#).
- **Crop Wavelength:** Specify the minimum and maximum wavelength used to crop the TOF 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

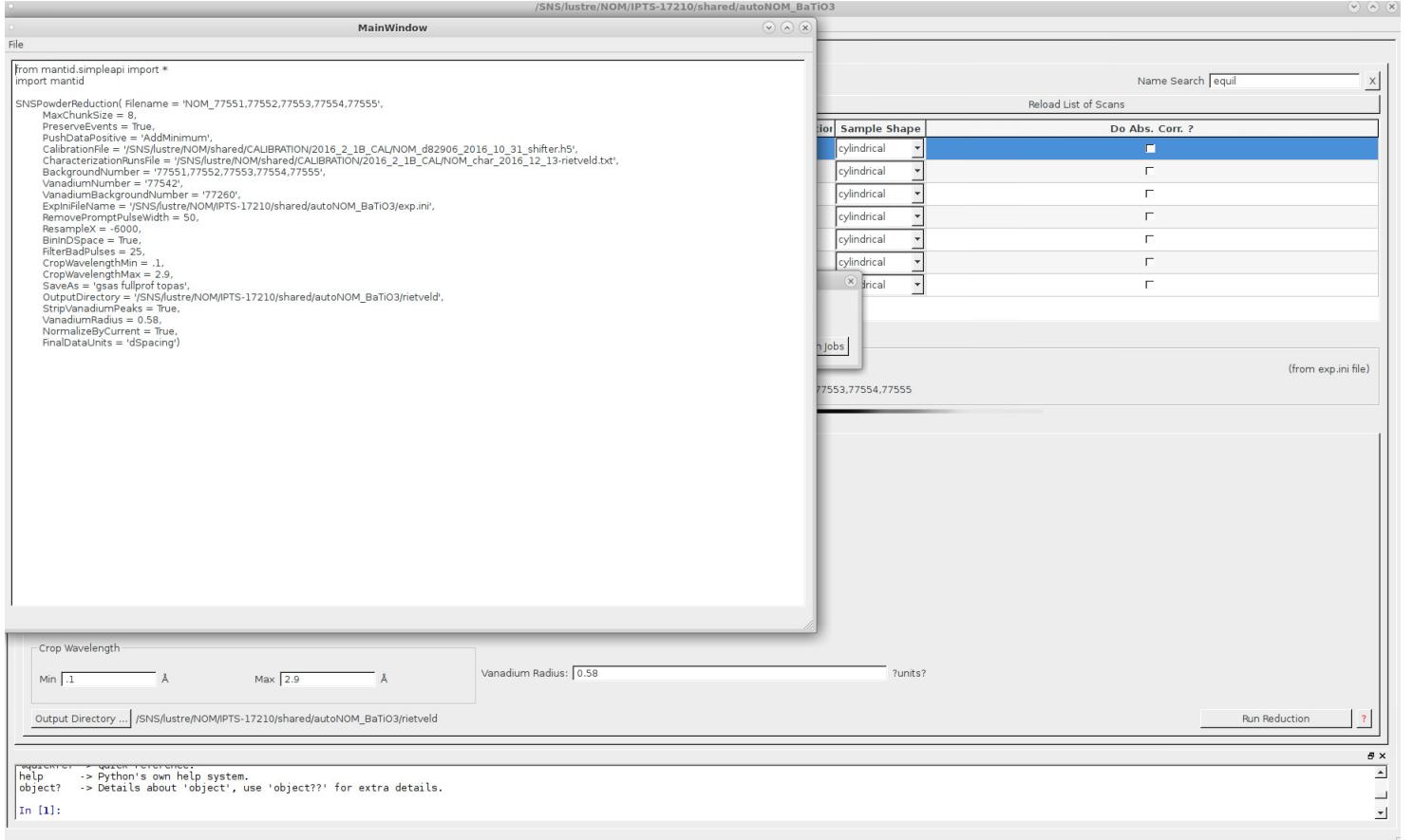
output directory will be placed. The directory will be named `rietveld` by default. It is recommended to place it inside the `autoNOM` directory or the parent `shared`. When you press the ***Output Directory*** button, you will be shown a file dialog box similar to the one below. we have already chosen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

### 4.3 Standard plot buttons

For all plot views in ADDIE, you will see a common button set on the bottom left that is standard. Here, we describe what each button does. The buttons are shown below:



The buttons and their functions are as follows. You can also hover over these buttons to get a description of what they do:

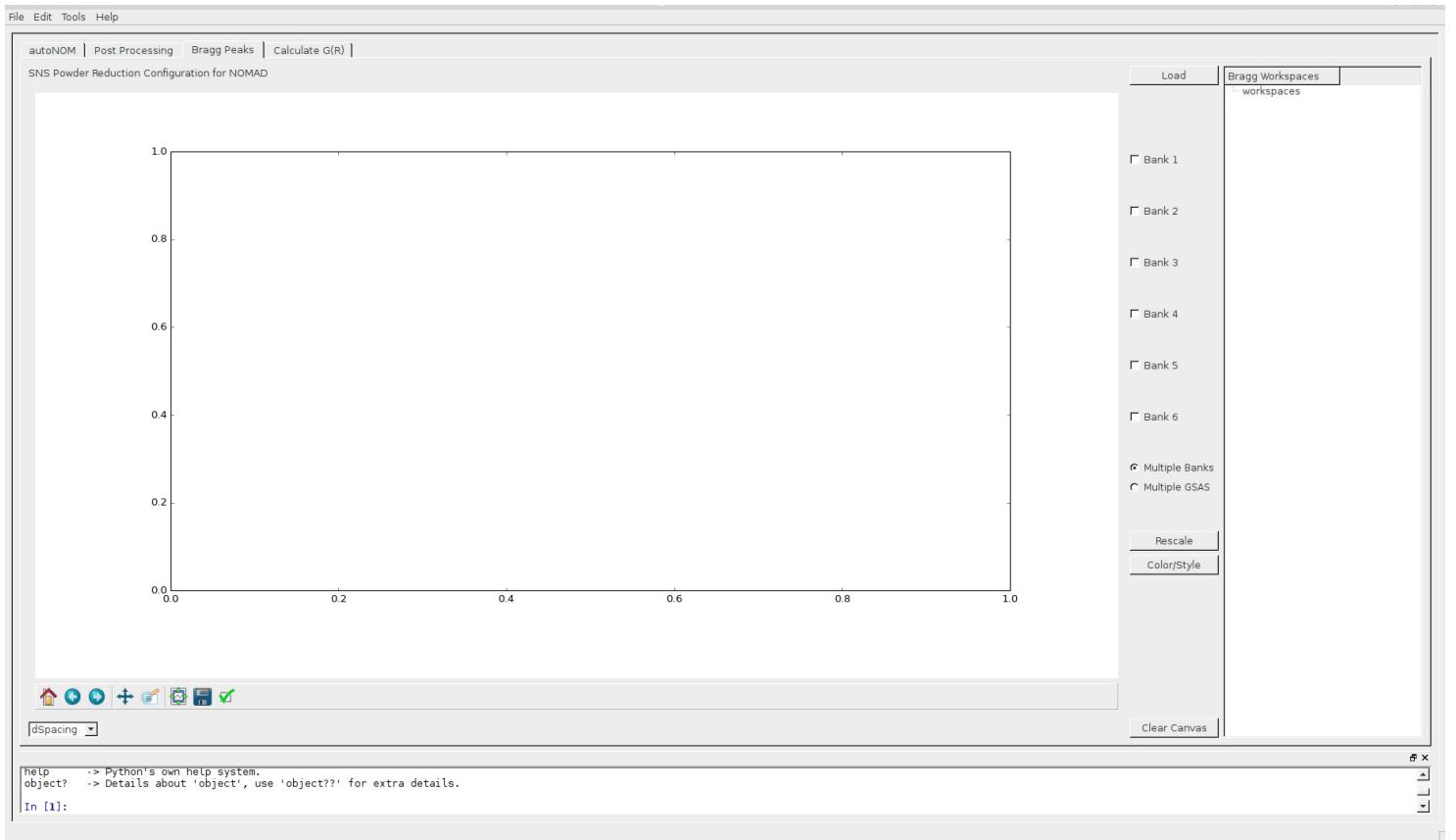
- **Home:** This allows you to reset the plot view to how it was initially when you loaded in the data. It is much like a "reset" button for the scale of the plot.
- **Back Arrow:** This will return to the previous view. If you have zoomed numerous times on the plot, this will take you to the last previous view.
- **Forward Arrow:** This will advance forward by one view. If you have zoomed numerous times on the plot and then went back, this will take you forward once more in your view.
- **Mutli-directional Arrows:** Enter Pan-mode. The left-click button will translate the figure in the plot view, the right-click will zoom the figure in the plot view **WARNING:** This conflicts with an option to manipulate the Legend. It can still work but typically we use the magnifying glass if we need to zoom the plot instead.
- **Magnifying Glass:** Allows you to box-select an area to zoom in on. Use the **Back Arrow** and the Home buttons to return to previous views.
- **Subplot Config:** This allows you to adjust the plot view to span more or less of the whitespace in the plot.
- **Floppy Disk:** This allows you to save the plot as a static image in a few different file formats. These can be viewed external from ADDIE. On the **Analysis** machine, you can use the **Eye of Mate** program that is available under the **Applications** drop-down on the top left.
- **check Box:** This allows you finer control over the figure options. You

can change the curve color, add markers, change labels of figures in the plot, change the minimum and maximum values of each of the axes, and also change the scales from linear to log and vice versa.

## 4.4 Visualize Bragg Diffraction

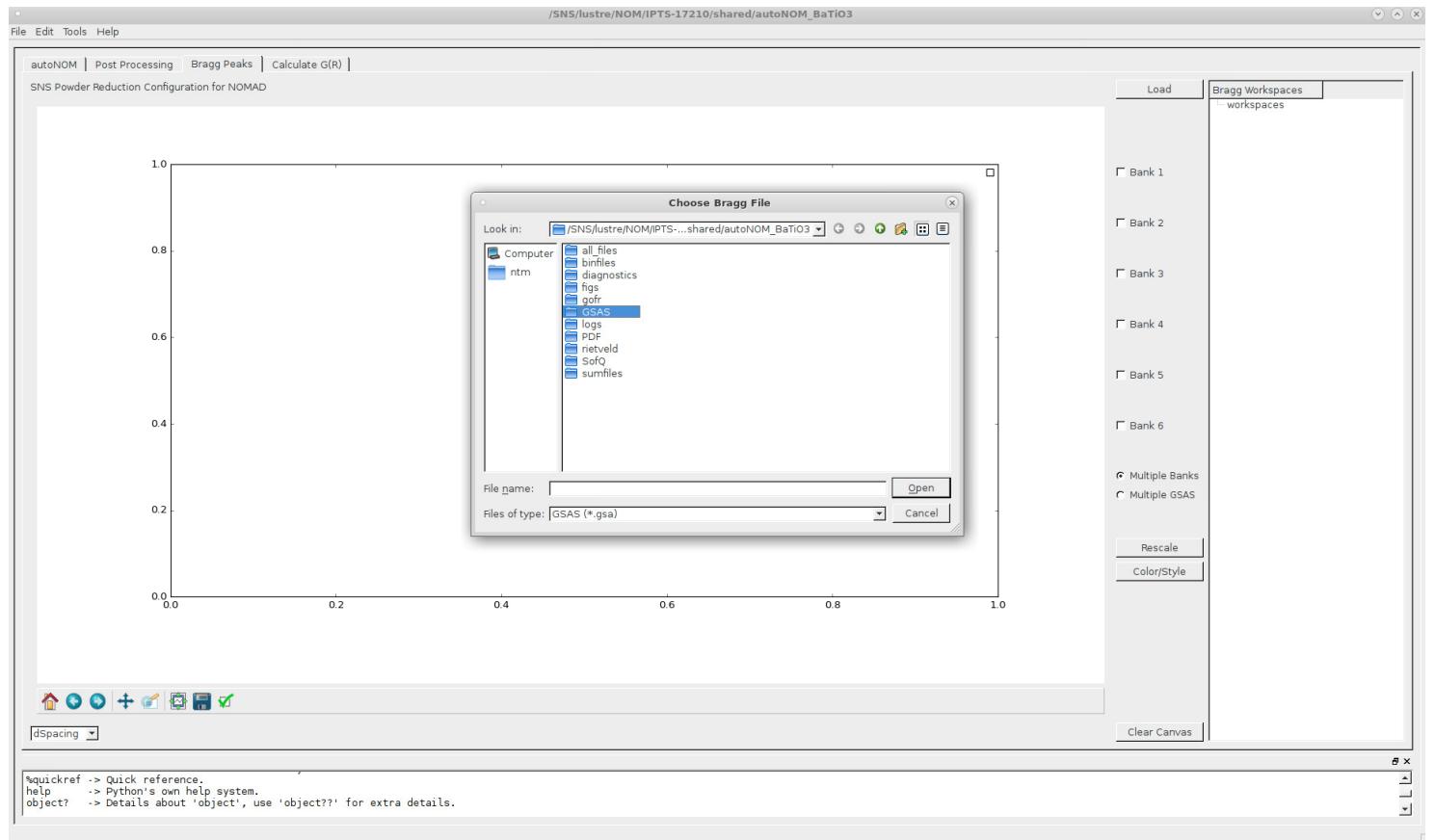
As individual runs or post-processed runs are completed, the output files will be placed in their respective directories specified in Table 4.1.5. The diffraction data is found in multiple directories: `GSAS`, `fullprof`, `topas`, and `rietveld`. Also, the `/SNS/NOM/IPTS-<your experiment ID>/autoreduce` directory will have diffraction data as well.

To visualize and plot the Bragg diffraction data, we use the **Bragg Peaks** tab shown below and we view the files located in the `GSAS` directory:

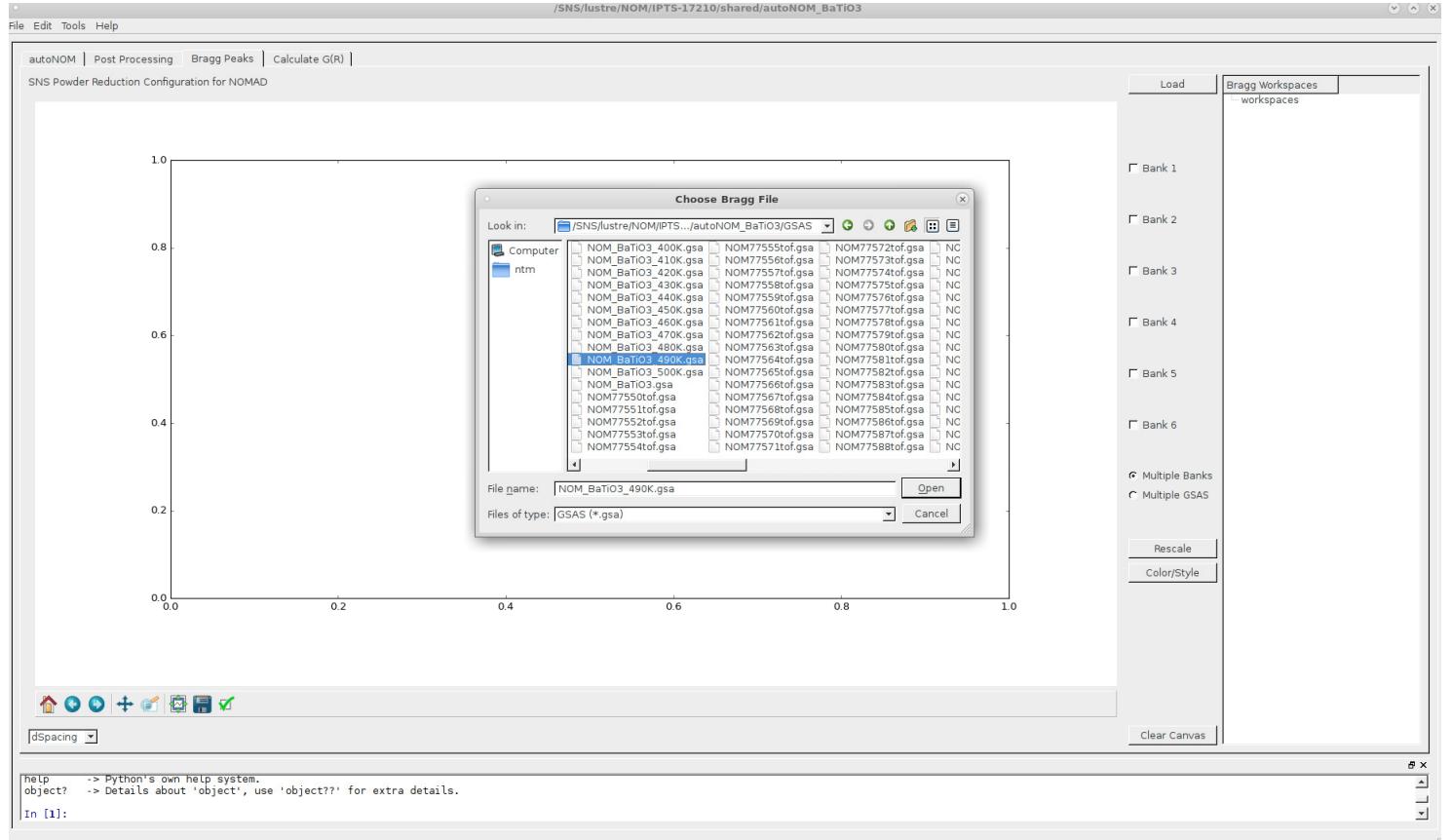


#### 4.4.1 Load Bragg data

First we need to load in diffraction data. Go to the top right and press the **Load** button. You should be presented with a file dialog similar to the one below:

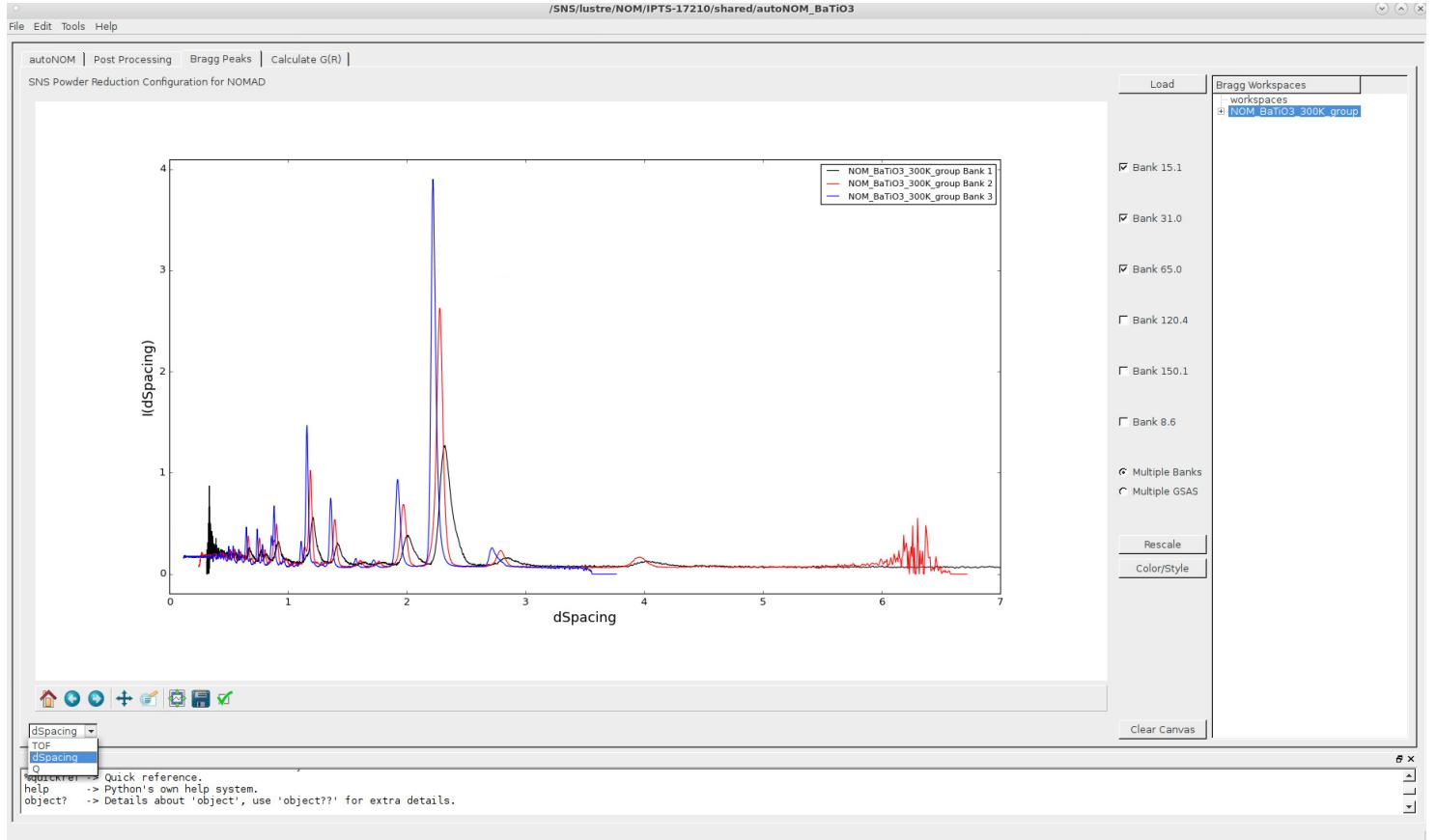


Double-click the **GSAS** directory to see the files that are available. When you press **Load**, you may actually start in the **GSAS** directory as well. From here, you can select individual runs, labeled as **NOM<run number>tof.gsa** or you can select post-processed runs such as summed files, labeled as **NOM\_<given title>.gsa**. An example is displayed below:



You can also select multiple individual runs while holding the **Ctrl** key or you can select a span of runs by holding the **Shift** key while selecting the runs. Once the runs are selected, press the **Open** button.

Below we show where we have loaded the summed run for 300K.



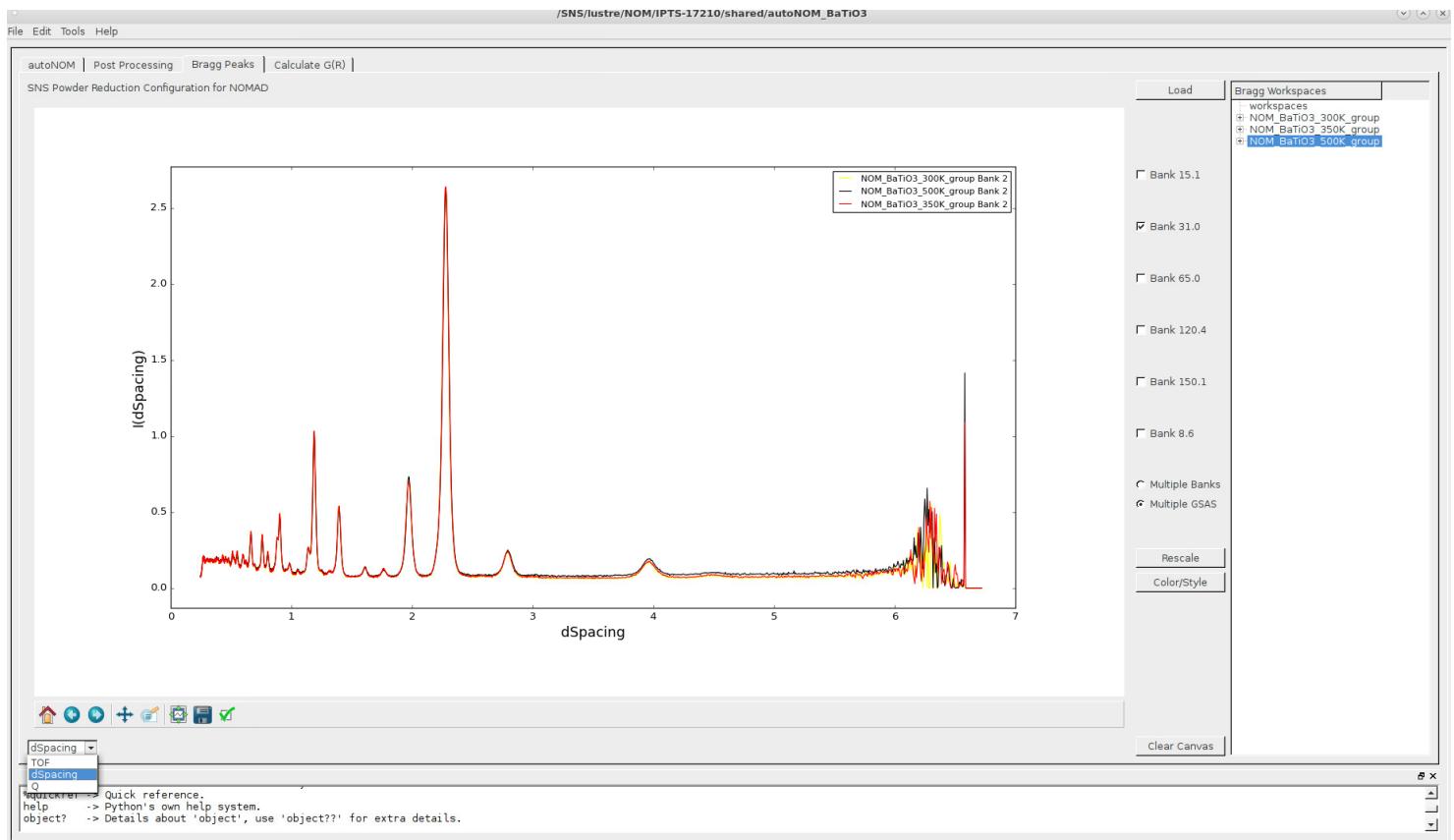
#### 4.4.2 Adjust Graphs

This tab has two modes to view the diffraction data from the banks: ***Multiple Banks*** and ***Multiple GSAS***.

- ***Multiple Banks***: In this mode, we can view diffraction data from different banks of the same run. We can select the banks to display on the right-hand side. We can select multiple different banks in this mode.
- ***Multiple GSAS***: In this mode, we can view diffraction data from different

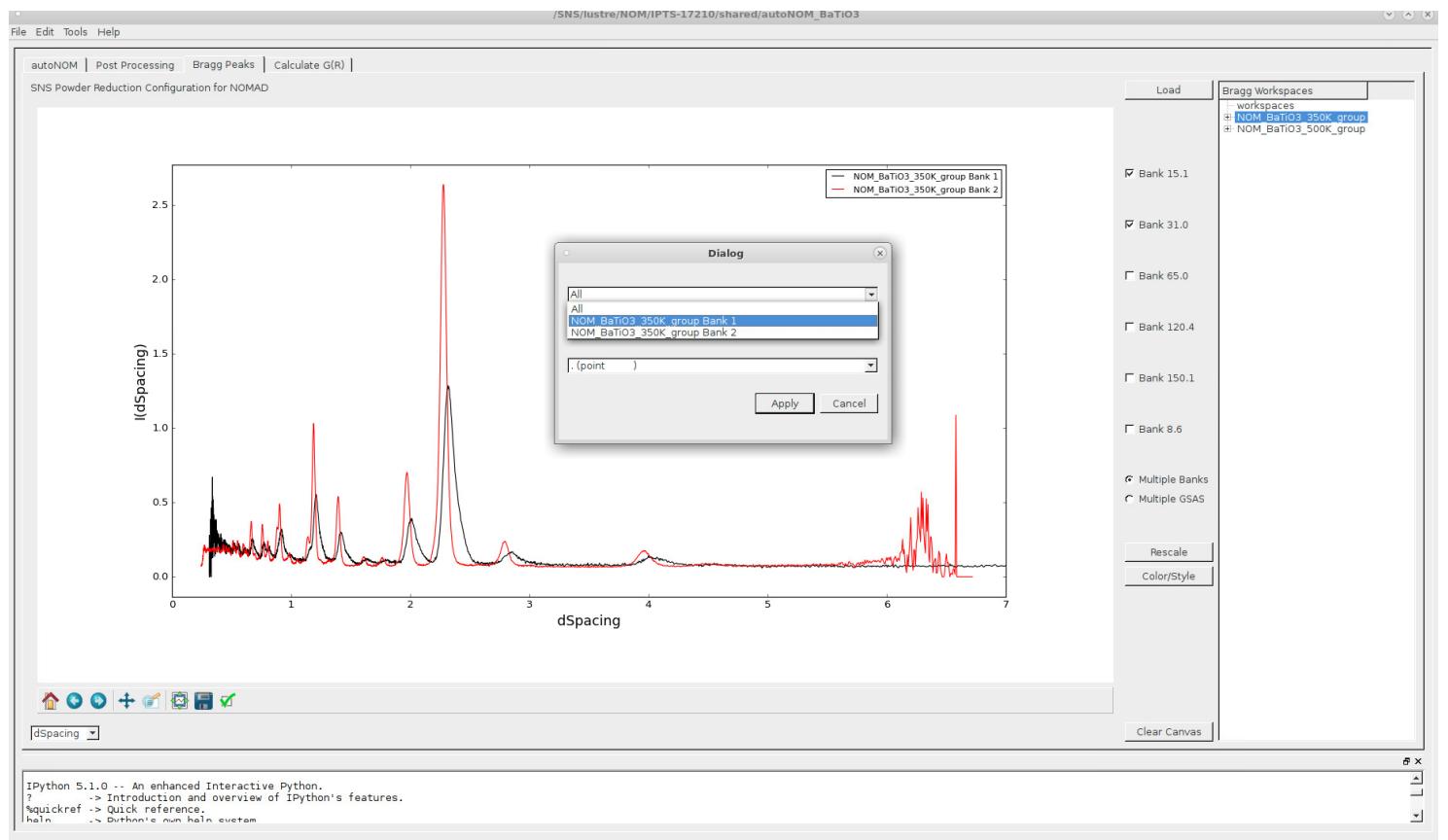
runs for a single bank. We can select the bank to display on the right-hand side. We can select only one bank at a time in this mode.

In Figure 4.4.2, we are in ***Multiple Banks*** mode and have three of the banks selected. When we load in more than one dataset, we can use ***Multiple GSAS*** mode. Below, we show where we have loaded in the 300K, 350K, and 500K data sets and have selected the 31.0 degree bank to view the data:



Under the bank and mode selection, we have the ***Rescale*** and ***Color/Style*** buttons. The ***Rescale*** button can be used to rescale the frame to better fit the data if the y-axis spans too far or not enough to capture the data. The ***Color/Style*** button can be used to change the display of the data in the plot. After pressing the ***Color/Style*** button, we are presented with a file dialog box.

We can select the workspace from the drop-down list we would like to change, shown below, and can change the color of the curve, add markers, and select the fill and edge color of the markers from the other drop-downs:

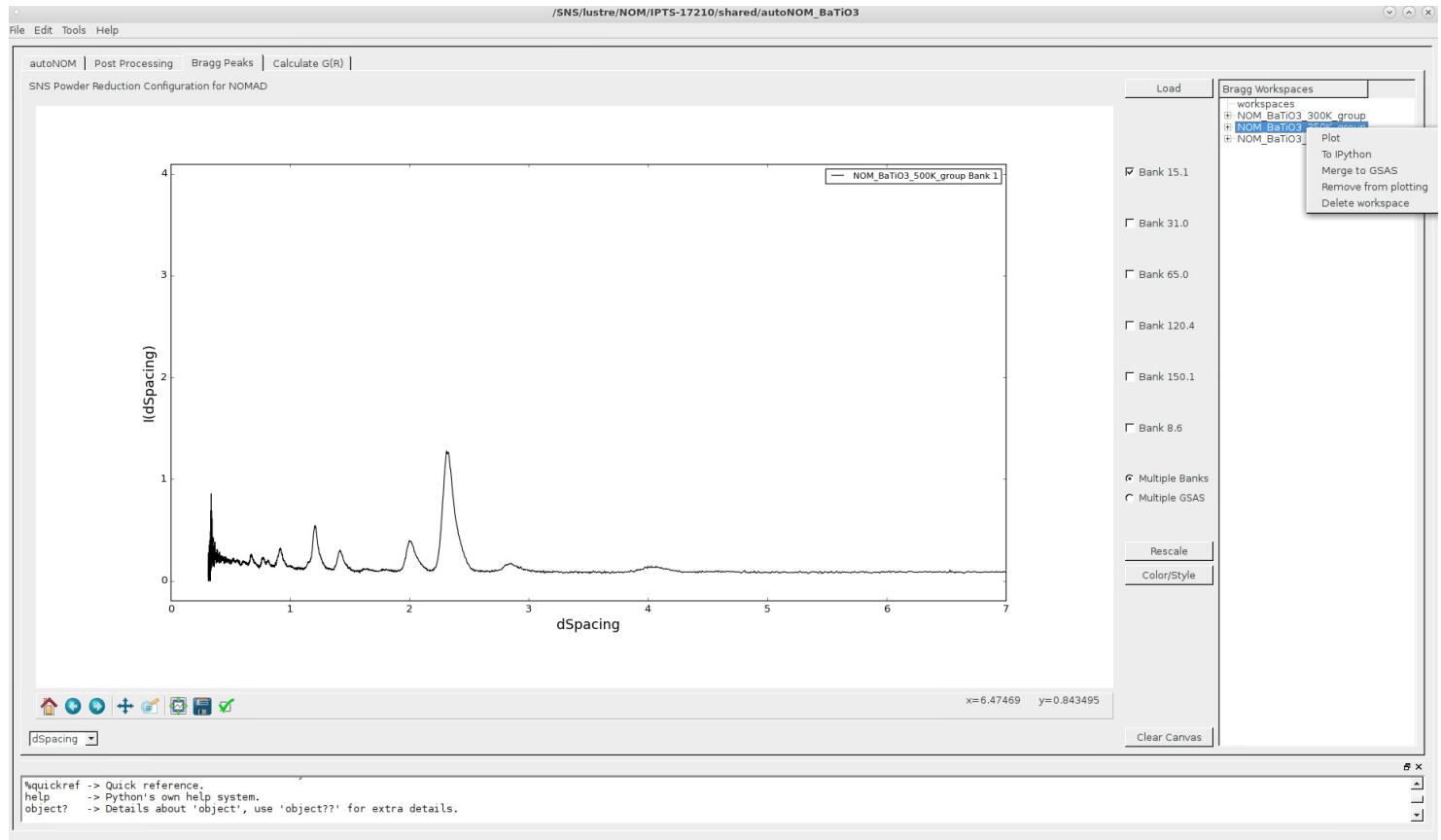


Under the ***Rescale*** and ***Color/Style***, we have the ***Clear Canvas*** button. This can be used to quickly clear the plot of all datasets and begin again.

You will also notice in the bottom left of the tab space that we can change the x-axis that we display the graph in. The choices are: ***TOF*** for time-of-flight, ***dSpacing*** for d-spacing (the default), and ***Q*** for momentum transfer. The graph will change accordingly.

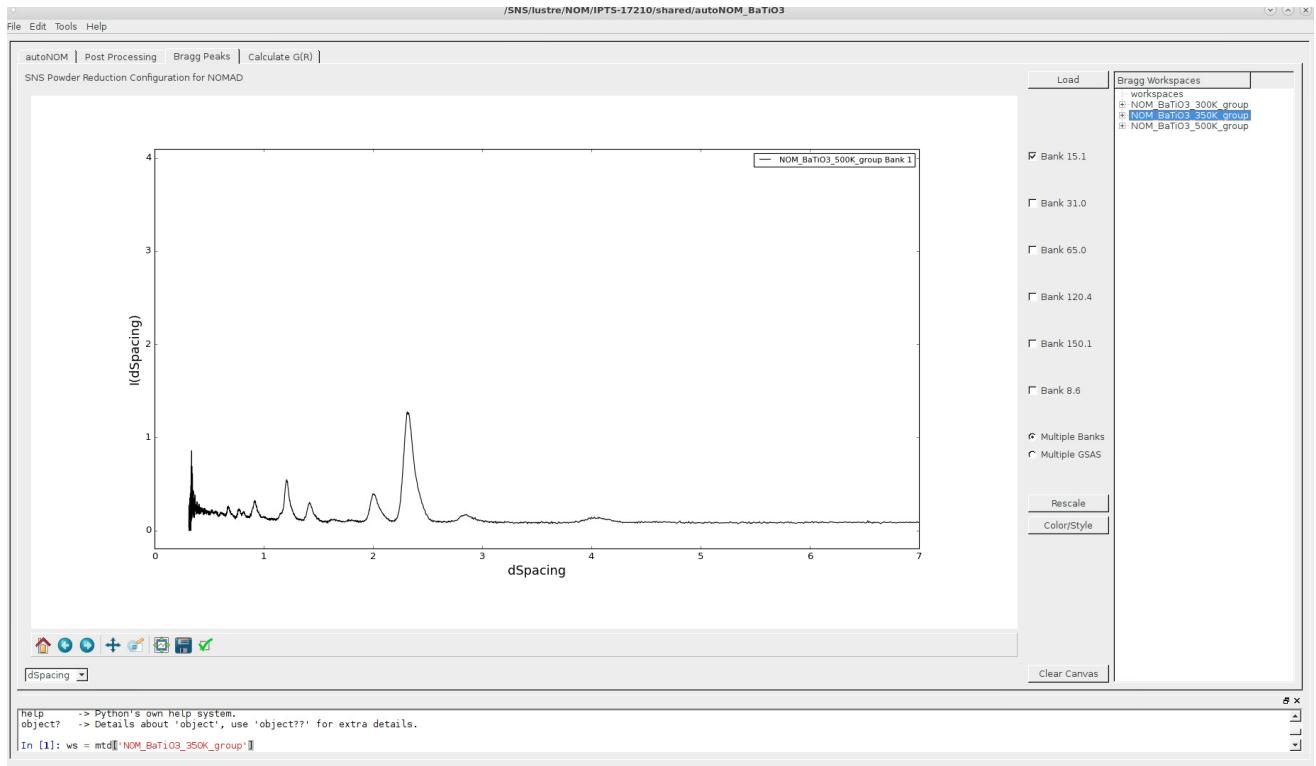
For each of the datasets that have been loaded, we have a ***Bragg Workspaces***

tree on the far right side. If you right-click on any of the workspaces, you will see the following options, demonstrated below:



From the options, you can do the following:

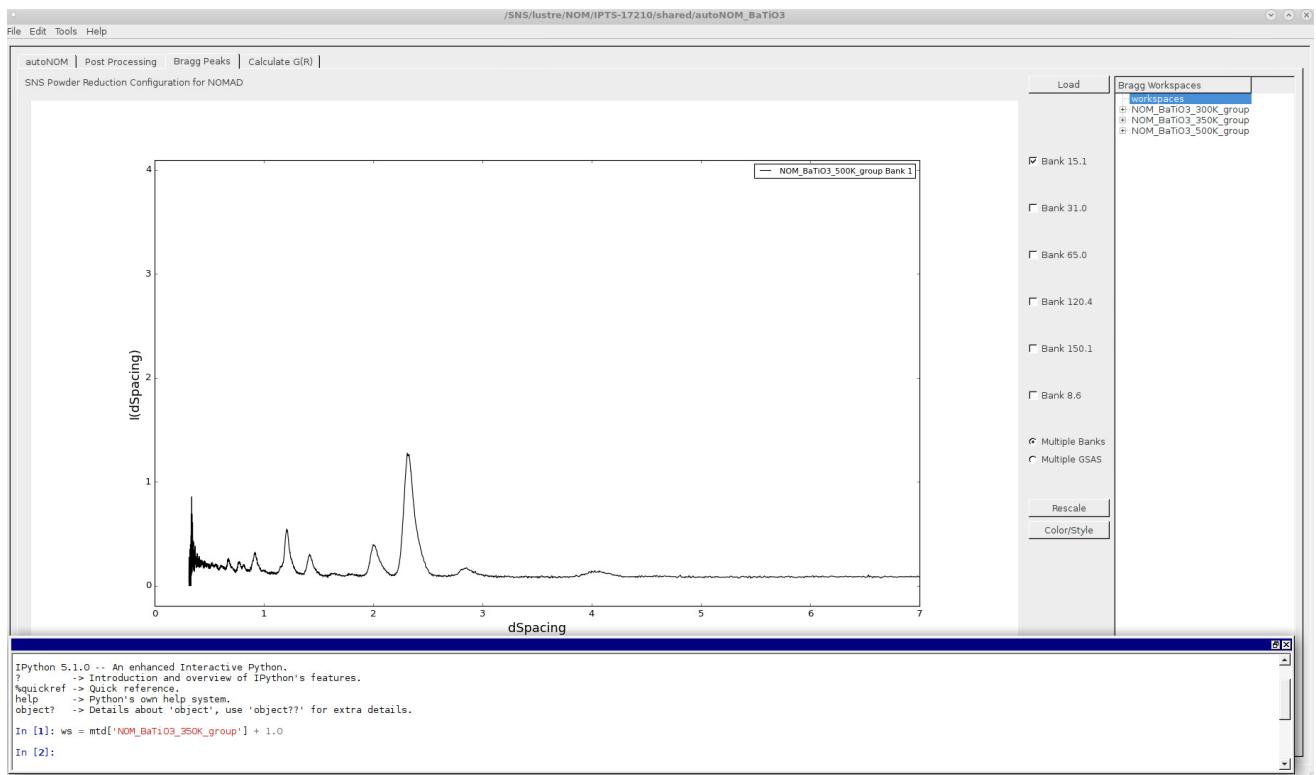
- **Plot:** Plot the selected workspace on the graph area.
- **To IPython:** Transfer the workspace to the IPython command line dock at the bottom. Here, you can script changes to the workspace and output a new workspace. If clicked, you will have something similar to what is shown below:



You can "undock" the IPython command line dock by pressing the double-window icon in the top right of the dock, shown below:



This will allow you to expand and contract the IPython command line dock. At anytime, you can redock by pressing the same double-window icon in the top right of the dock:



- **Merge to GSAS:** Will give a merged GSAS output file of the banks.

- **Remove from plotting:** Removes dataset from the plot.

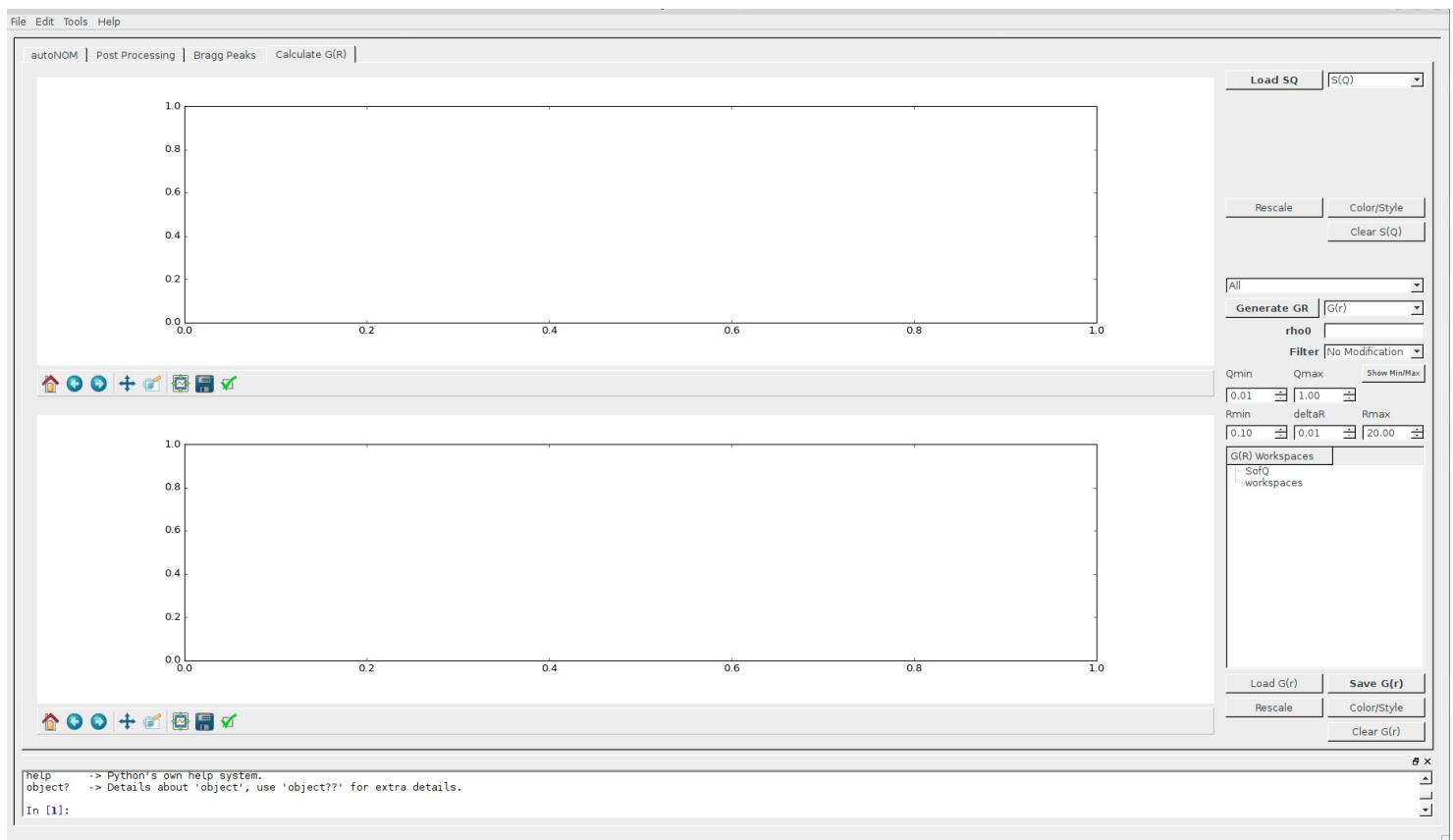
- **Delete workspace:** Deletes the dataset from the **Bragg Workspaces** tree.

To change the legend, in case it is in the way or masking data, you can right-click inside any of the plot areas and either reduce the font of the text, increase the font of the text, or hide the legend all together.

## 4.5 Visualize $S(Q)$ and $G(r)$

As individual runs or post-processed runs are completed, the output files will be placed in their respective directories specified in Table 4.1.5. The  $S(Q)$  data is found in the `SofQ` directory and the real-space data is found in the `gofr` and `PDF`.

To visualize and plot both sets of data (reciprocal-space and real-space), we use the *Calculate G(r)* tab shown below:

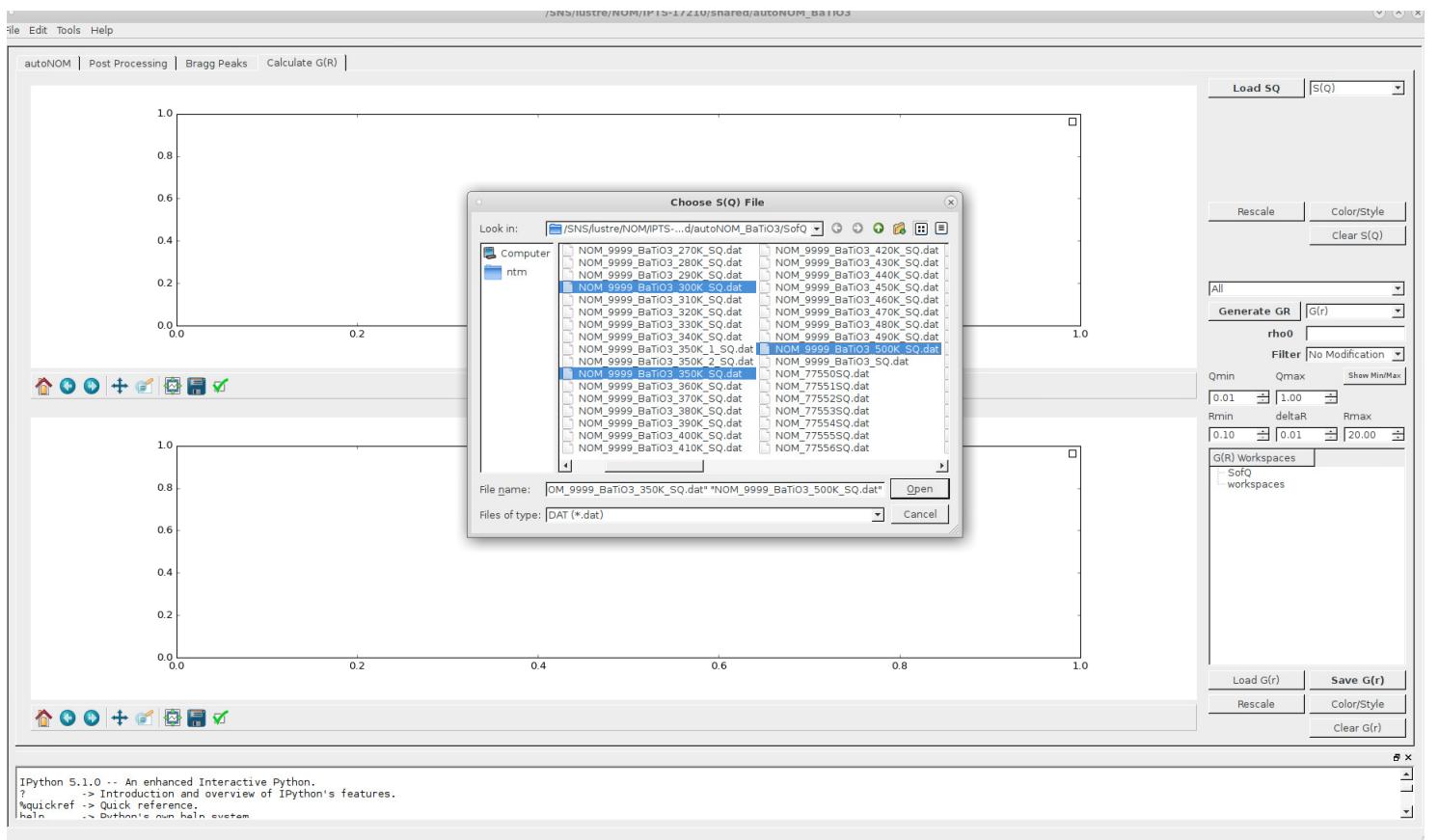


A note on how the two plots work: When  $S(Q)$  data is loaded in, the Fourier transform is calculated automatically and the corresponding  $G(r)$  is displayed in the corresponding plot. Thus, ADDIE allows one to simultaneously view both

the  $S(Q)$  and corresponding  $G(r)$  and also adjust and refine both datasets in an "on-the-fly" manner.

#### 4.5.1 Load $S(Q)$ data

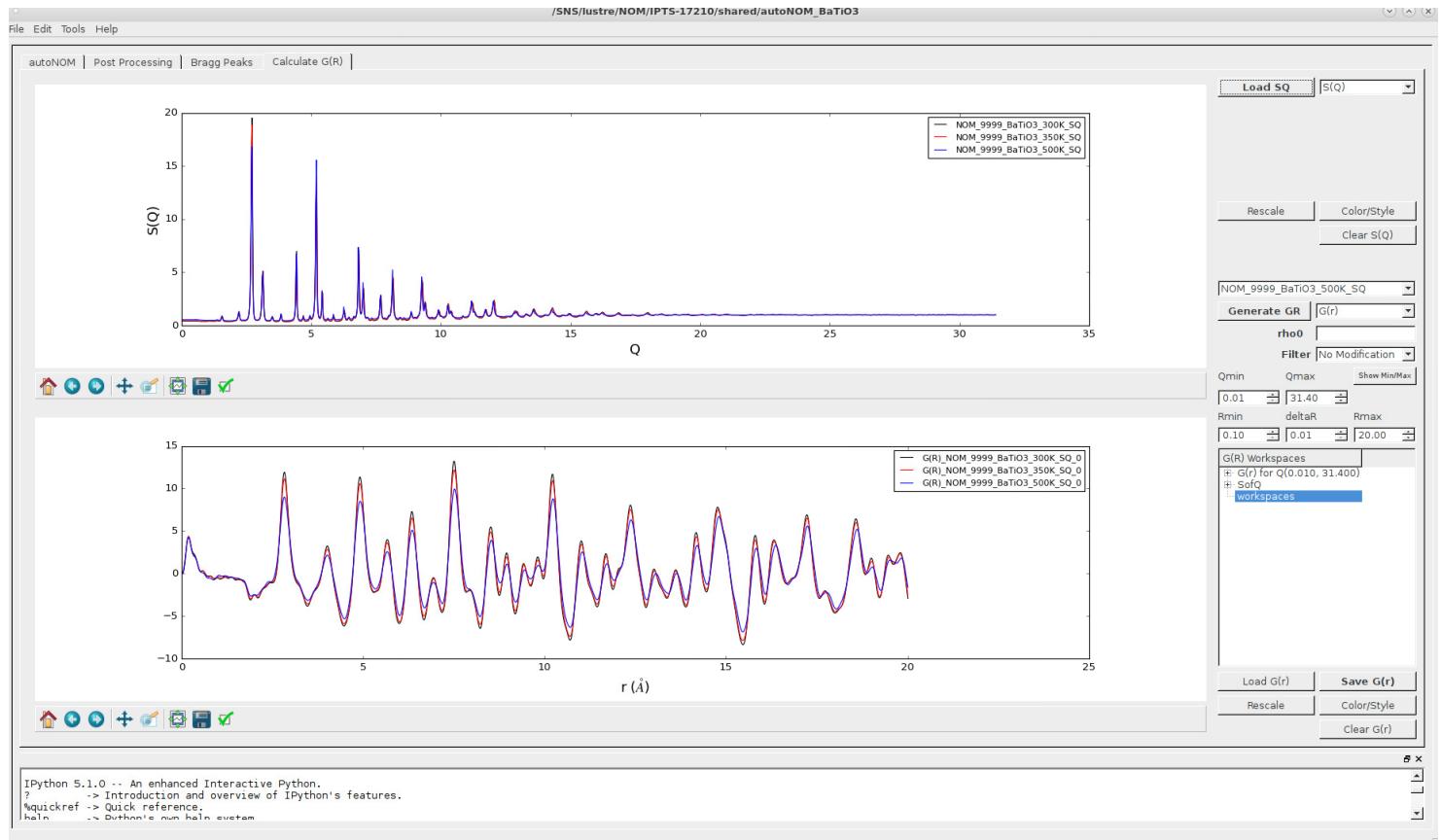
First load in  $S(Q)$  datasets. Go to the top right and press the ***Load SQ*** button. You should be presented with a file dialog similar to the one below:



If you are not in the **SofQ** directory, double-click the **SofQ** directory to see the files that are available. From here, you can select individual runs, labeled as **NOM\_<run number>SQ.dat** or you can select post-processed runs such as summed

files, labeled as `NOM_9999_<given title>.SQ.dat`.

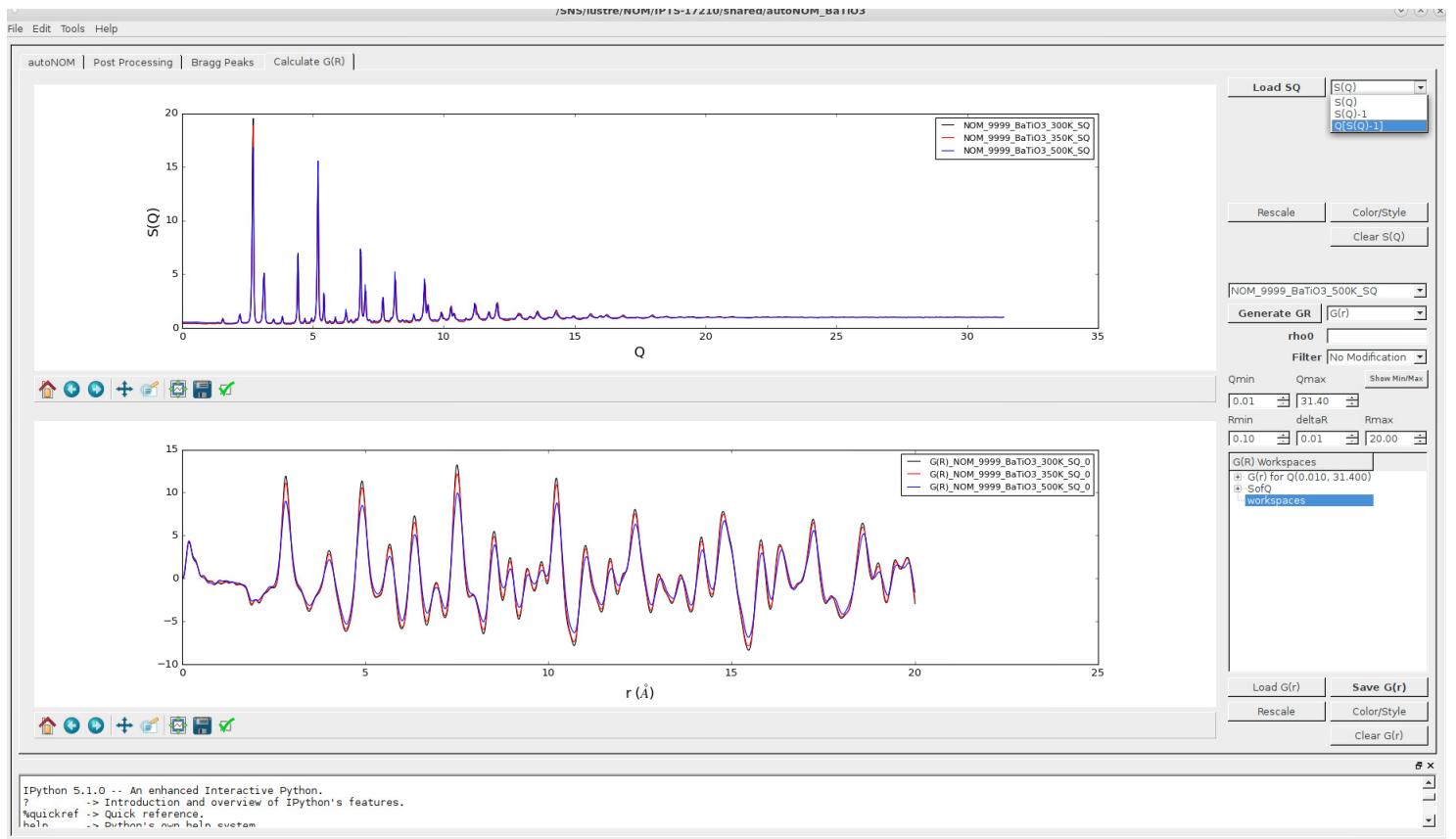
You can also select multiple individual runs while holding the **Ctrl** key or you can select a span of runs by holding the **Shift** key while selecting the runs. Once the runs are selected, press the **Open** button. For our example above, we get the following displayed:



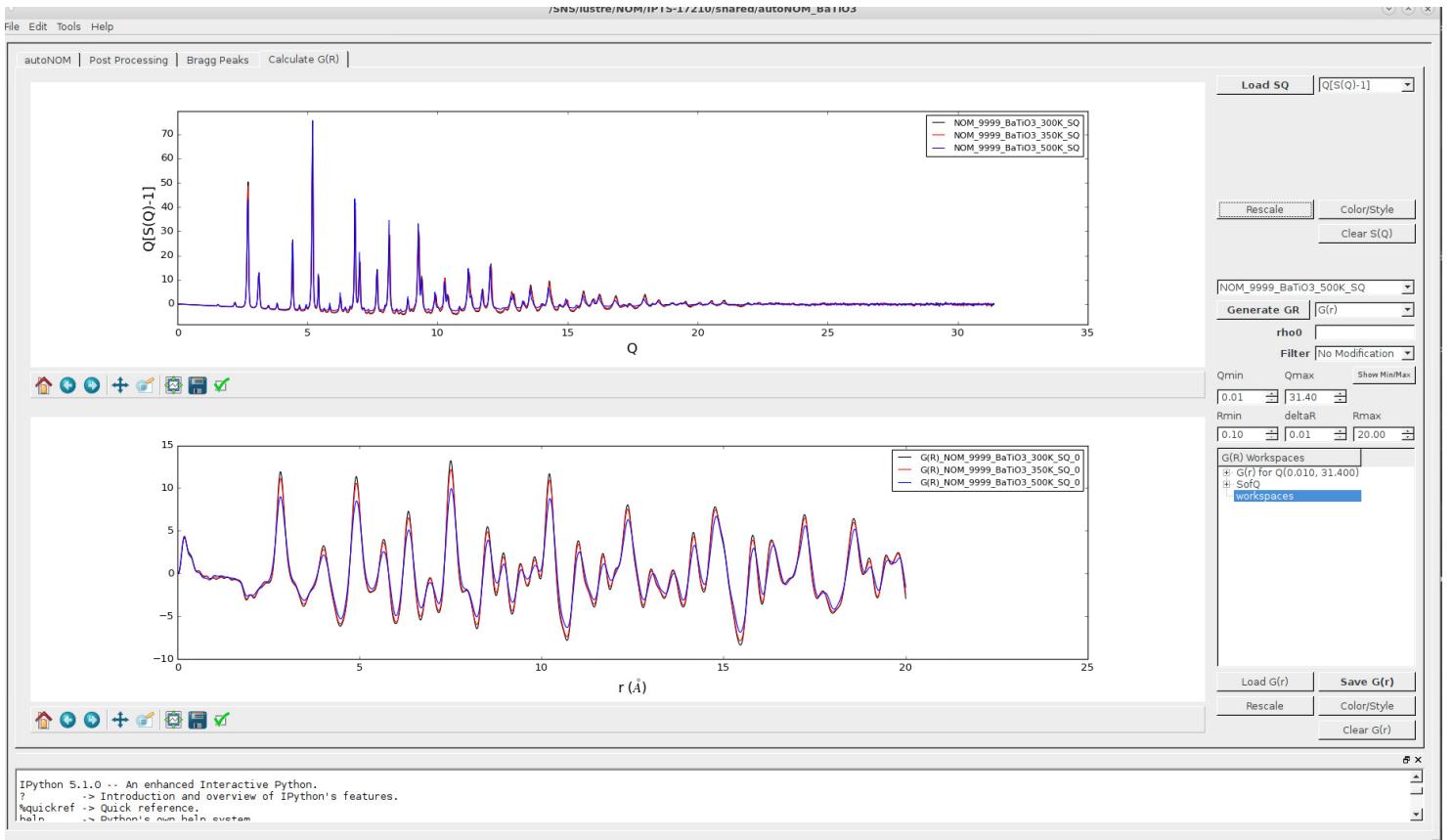
We can see all three datasets were loaded and the Fourier transform data is displayed as well, based on the current options set for the transform, described more below.

### 4.5.2 Adjust $S(Q)$ graphs

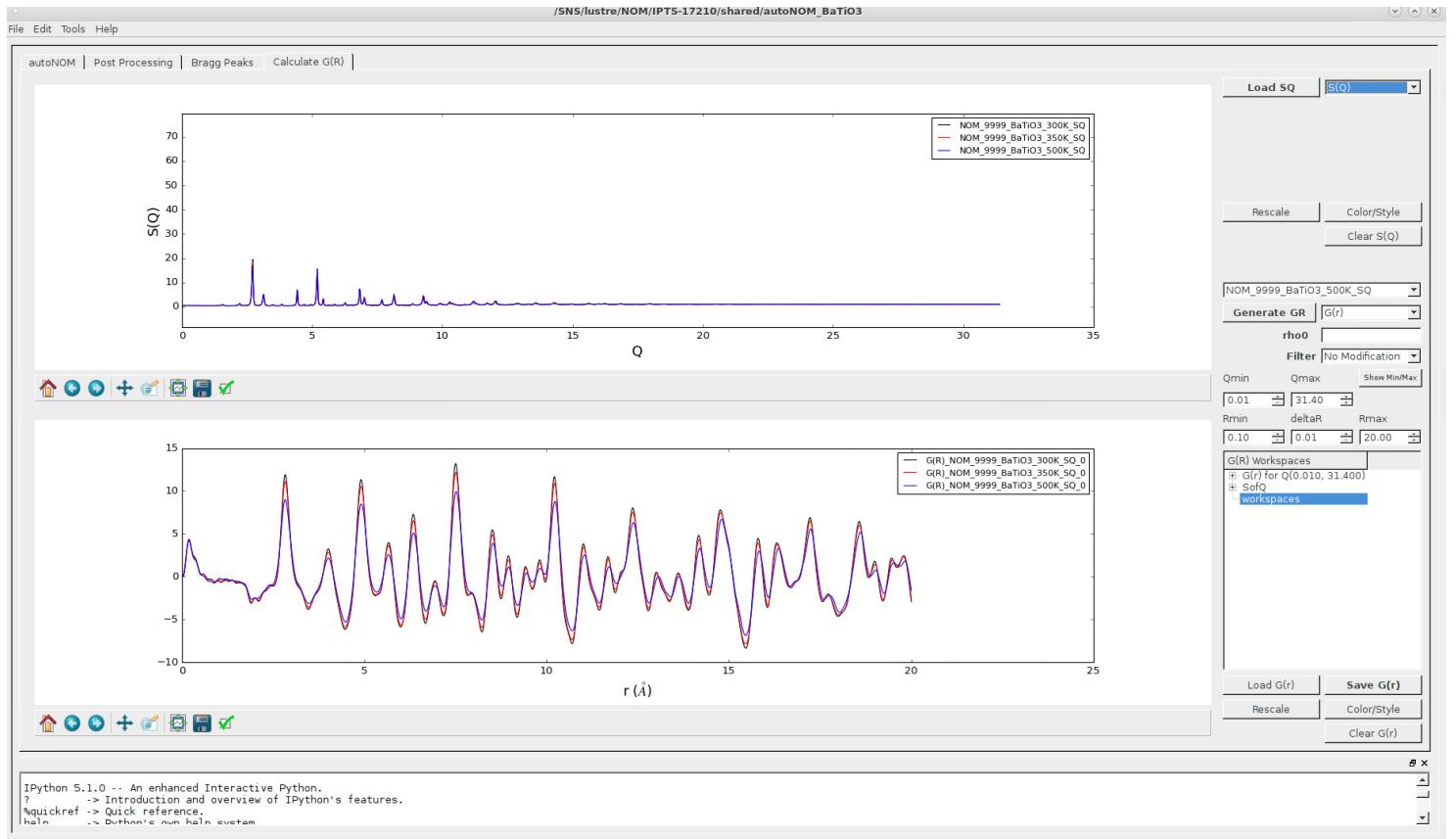
On the top right, next to the **Load SQ** button, we can change the x-axis of the reciprocal-space plot. We can choose from  $S(Q)$ ,  $S(Q)-1$ , and  $Q[S(Q)-1]$ , shown below:



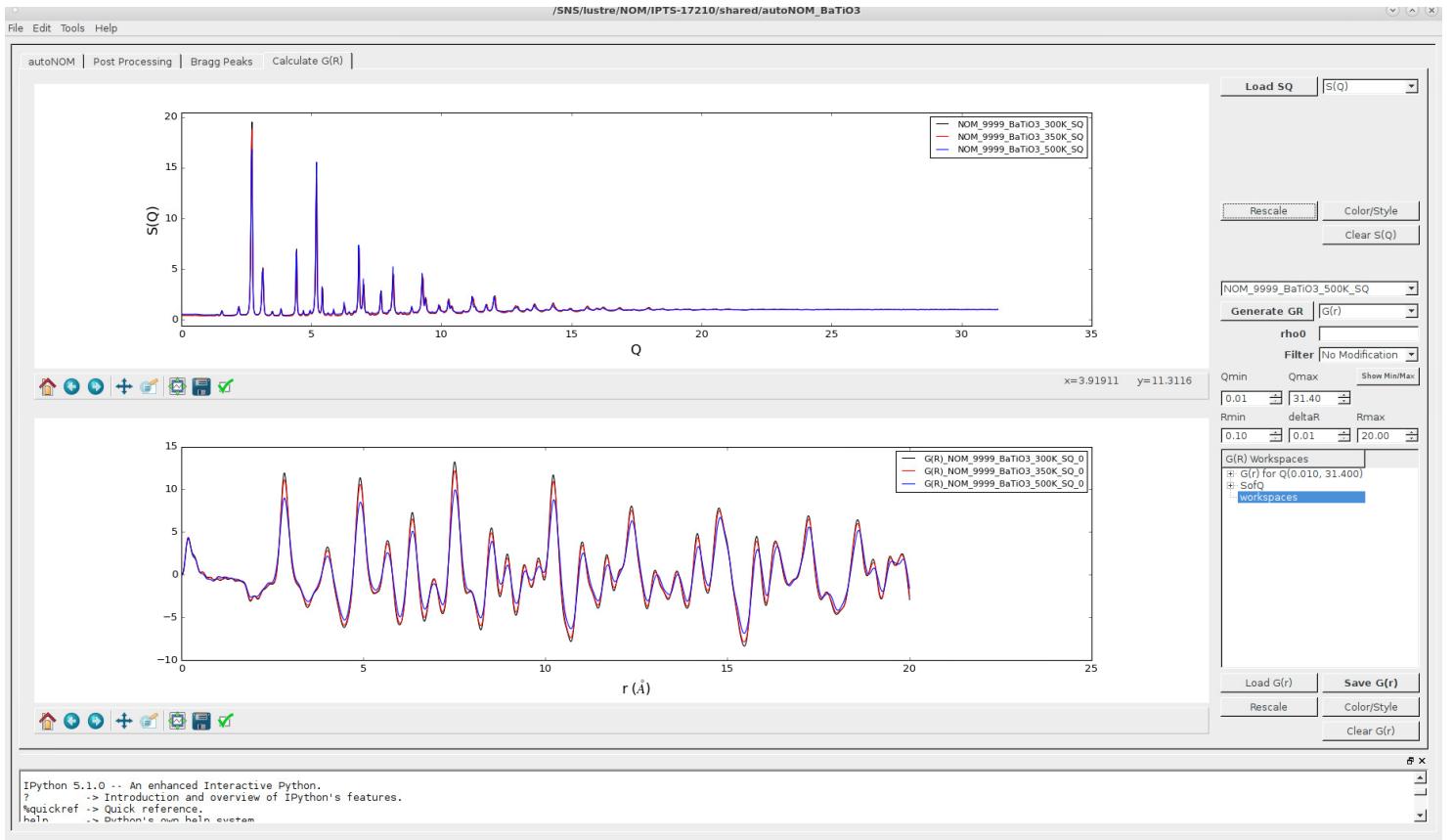
Selecting the  $Q[S(Q)-1]$  option will produce a plot view like the one below:



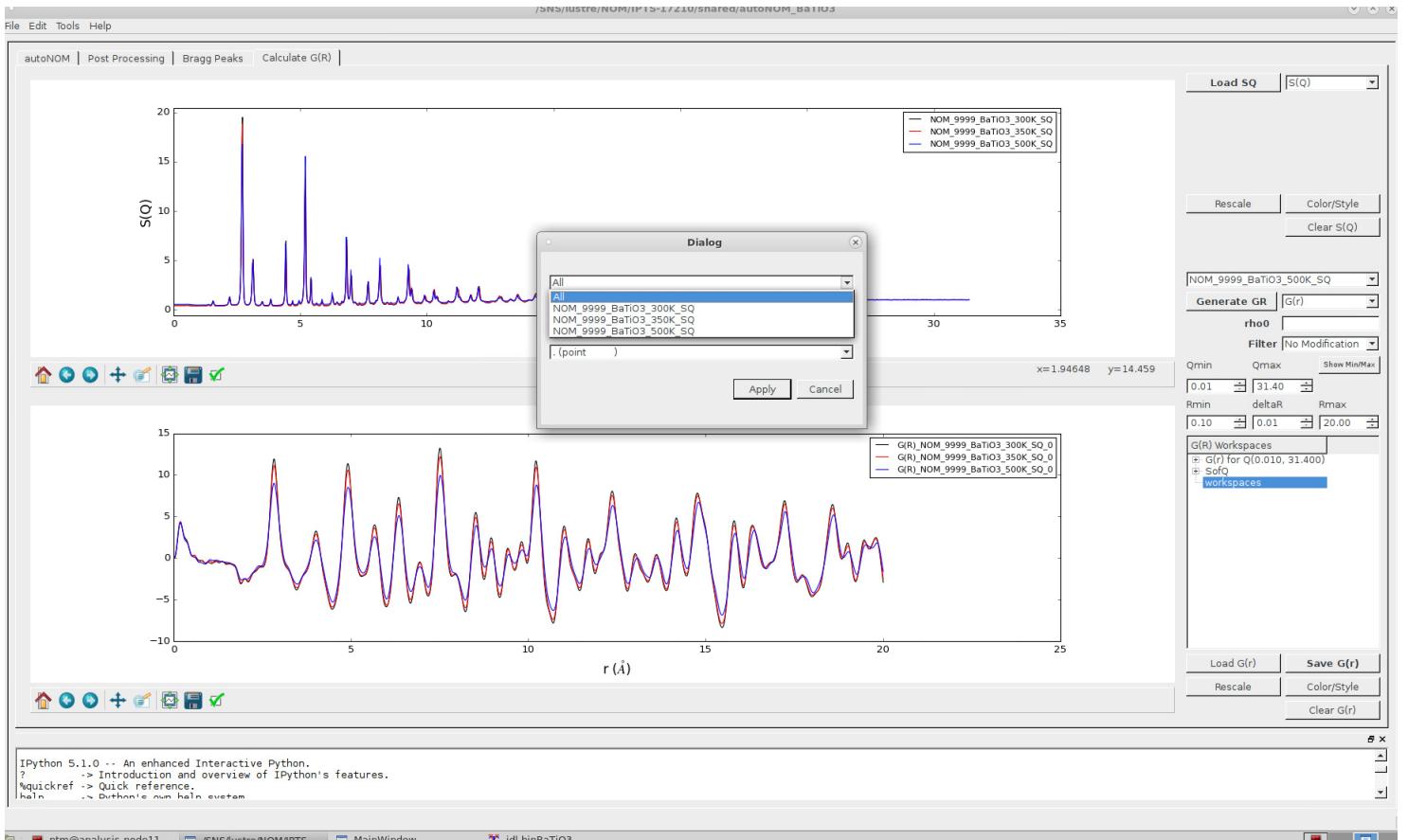
Below this, we have the **Rescale** button. If we change the previous drop-down back to  $S(Q)$ , we get the following in the display:



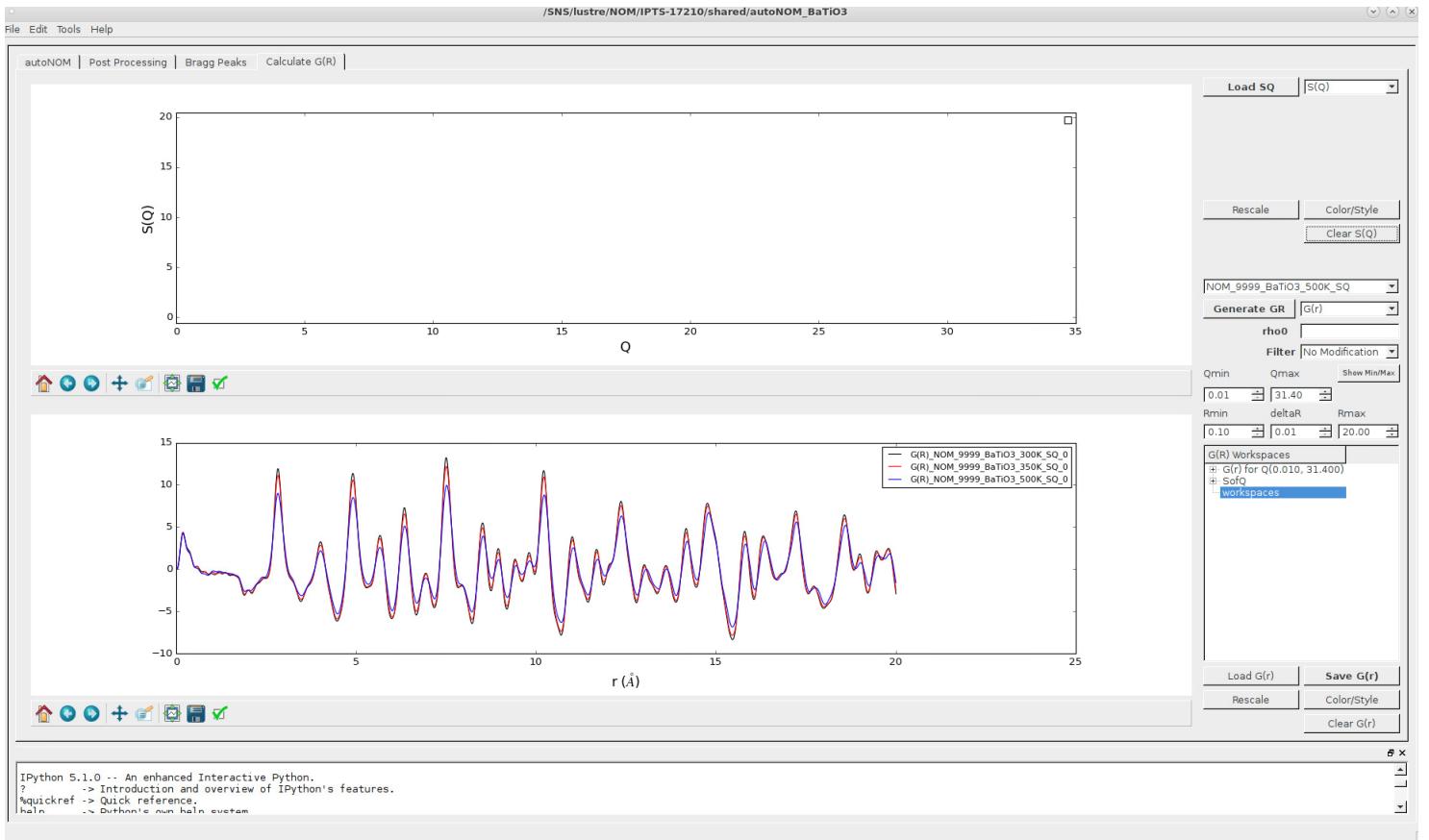
Clearly, the figure needs to be rescaled to display the data properly. Clicking the **Rescale** button, we get back to the previous state for the  $S(Q)$  data, as shown below:



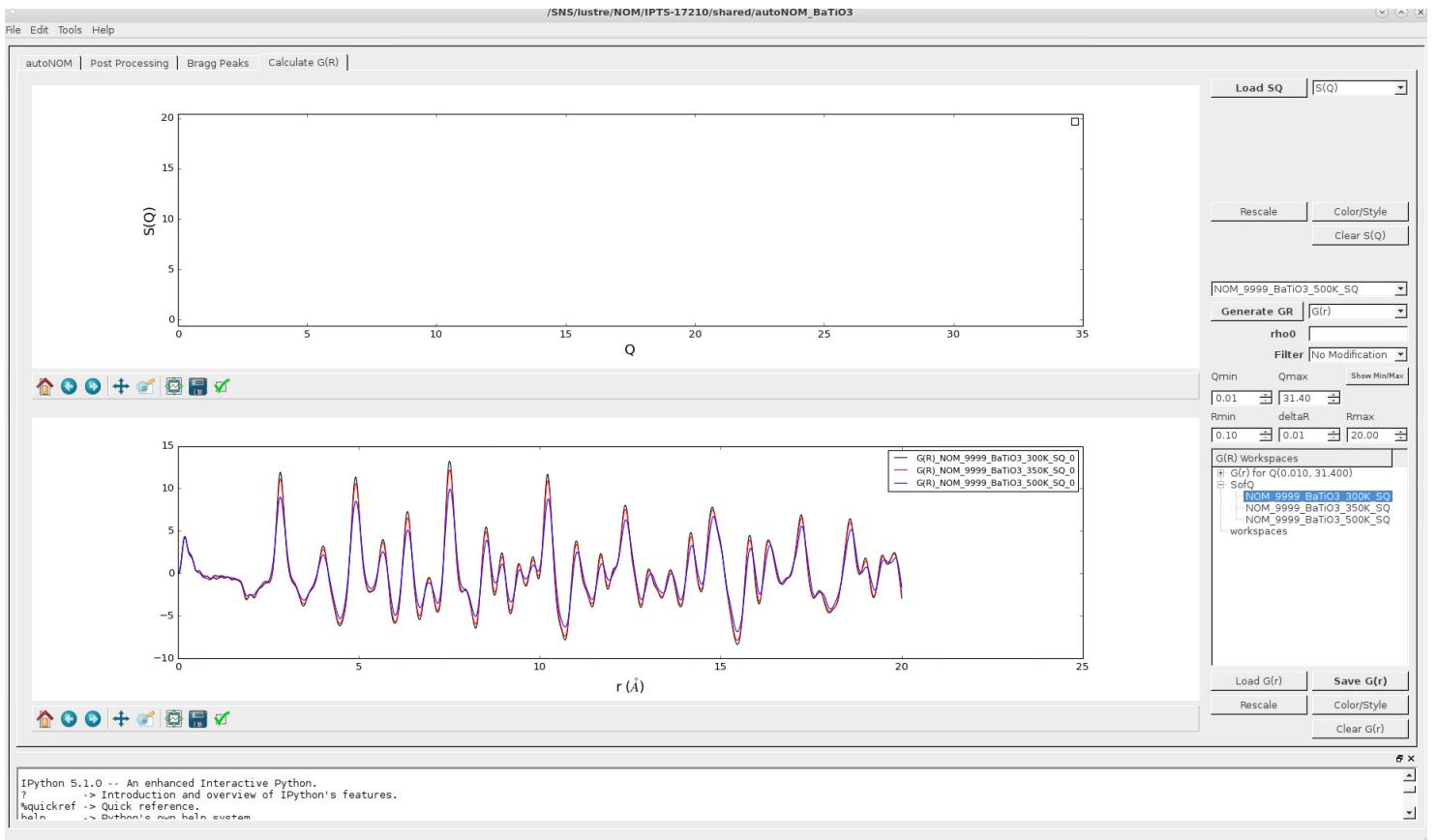
The ***Color/Style*** button can be used to change the display of the  $S(Q)$  data in the plot. After pressing the ***Color/Style*** button, we are presented with a file dialog box. We can select the workspace from the drop-down list we would like to change, shown below, and can change the color of the curve, add markers, and select the fill and edge color of the markers from the other drop-downs:



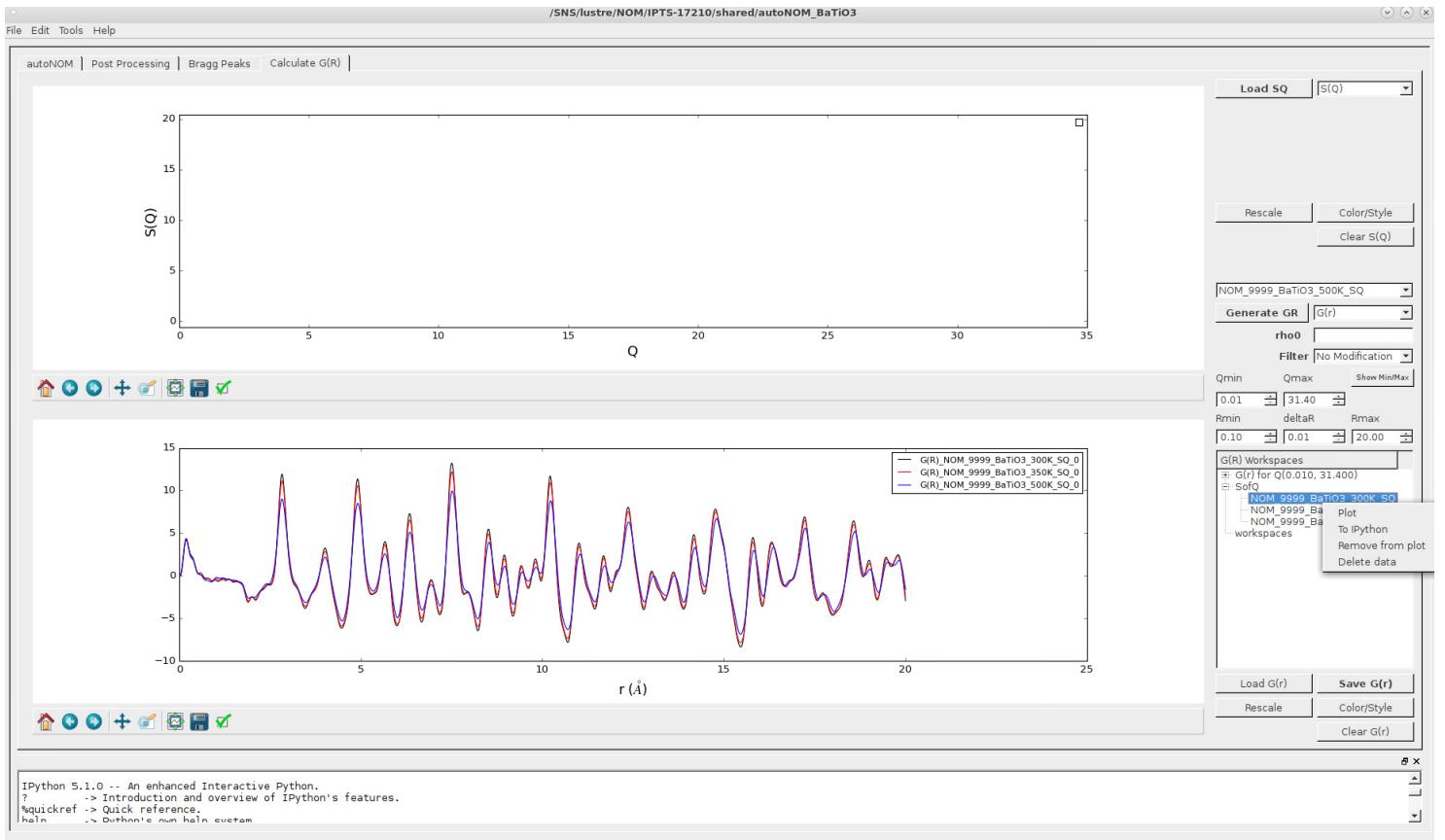
The **Clear S( $Q$ )** button can be used to clear the plotted reciprocal space data sets from the plot view. The datasets are still available to replot in the **Workspace Tree**. If we press this from the previous state, we end up with the following below:



In the **Workspace Tree**, we can expand the SofQ parent node and see the datasets still available. In the following, we see the datasets are still available even though we cleared the plot view previously:

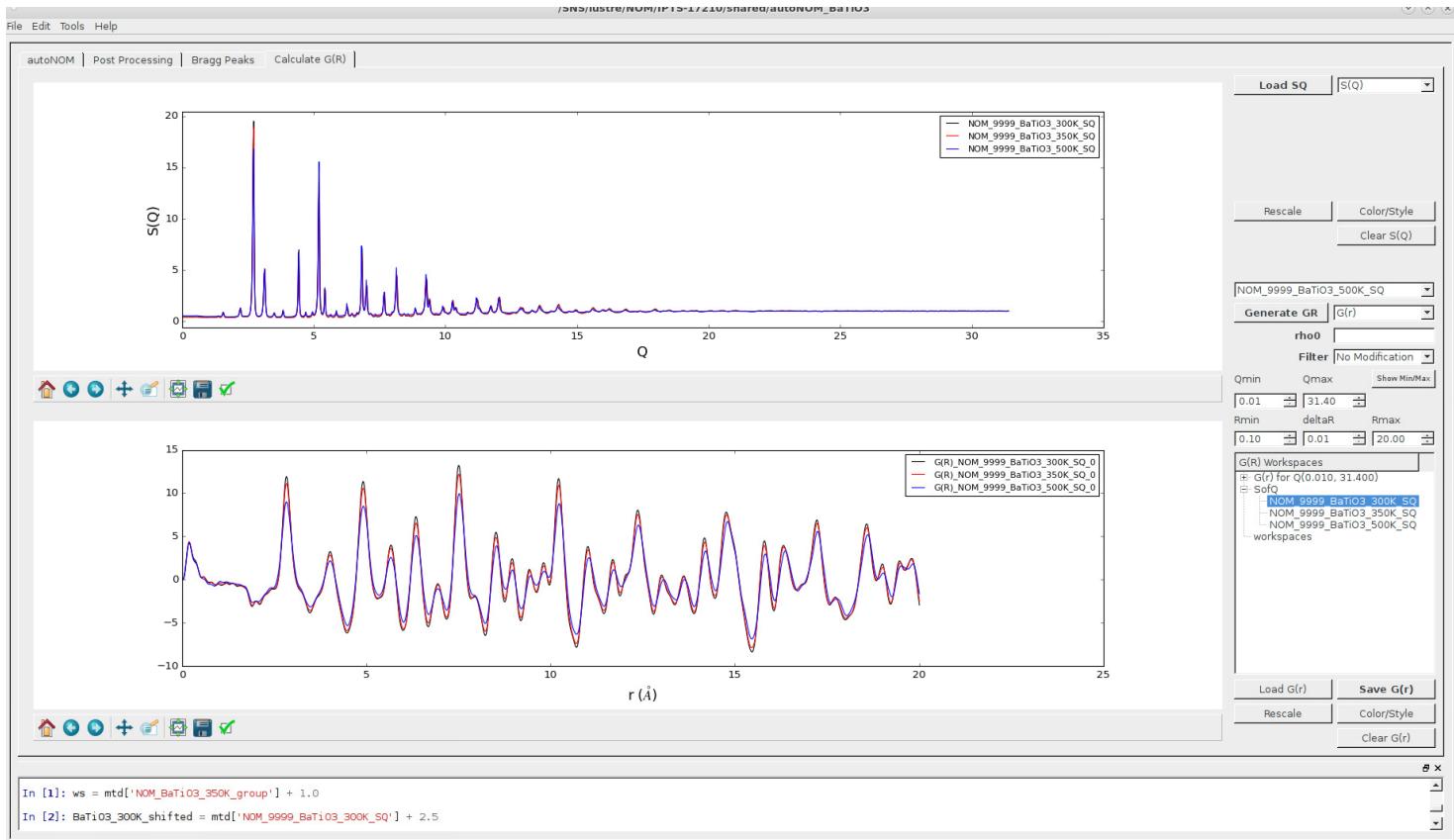


Right-clicking any of the data sets in the SofQ workspace tree will give the following options shown below:



These options are as follows:

- **Plot:** This will plot the dataset in the  $S(Q)$  plot view.
- **To IPython:** Transfer the workspace to the IPython command line dock at the bottom. Here, you can script changes to the workspace and output a new workspace. If clicked, you will have something similar to what is shown below. Here, we have already typed in to add a 2.5 shift:



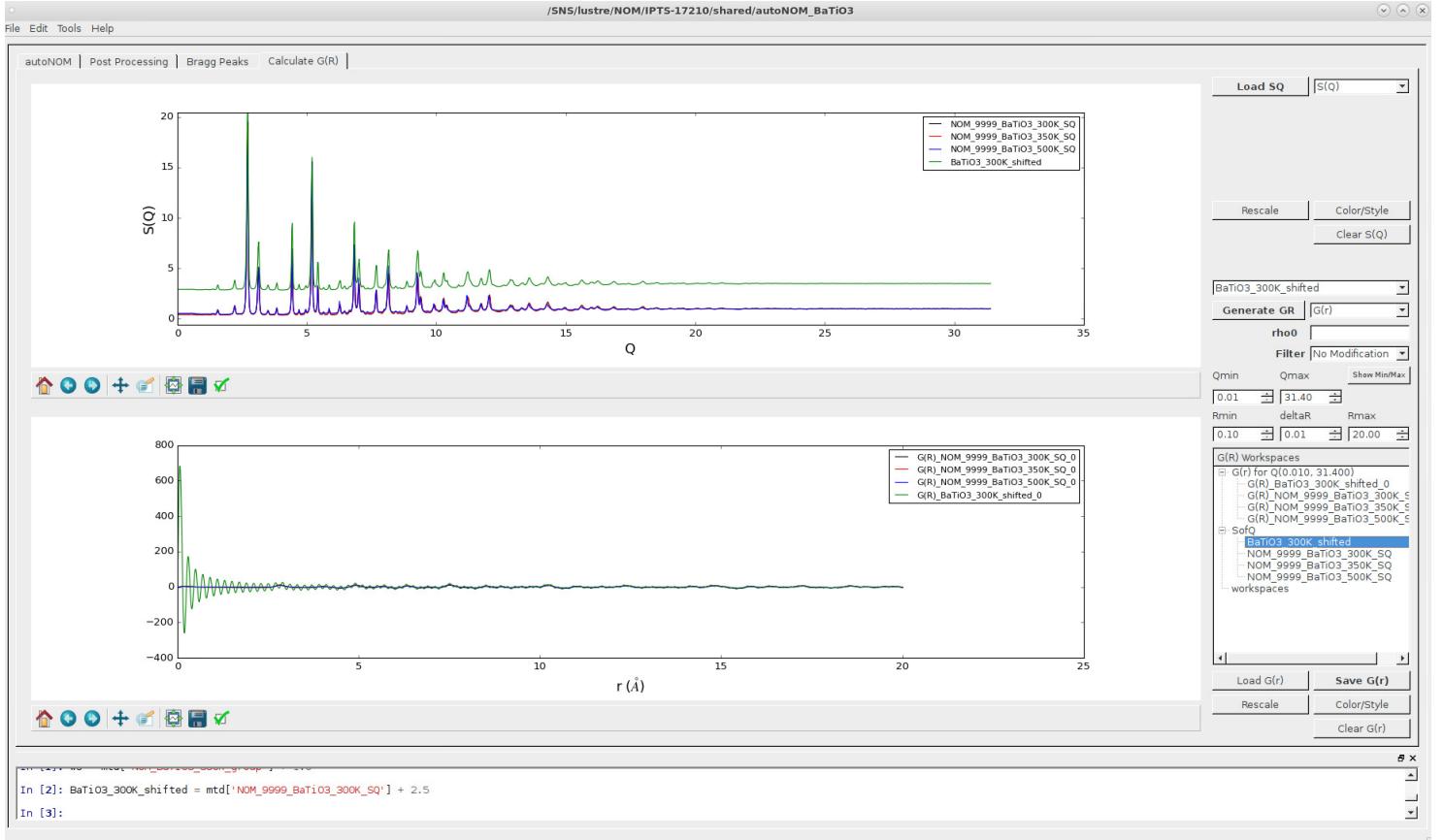
If we name this new workspace "BaTiO3\_300K\_shifted" and execute the command in the IPython prompt, we will get a new SofQ workspace with this title in the **Workspace Tree**. We show below the highlighted workspace in the tree and also have added the plot to the  $S(Q)$  plot area:



You can dock and undock the IPython command line prompt by selecting the double-window icon on the top right of the dock, explained previously in the **Bragg Peak** tab section.

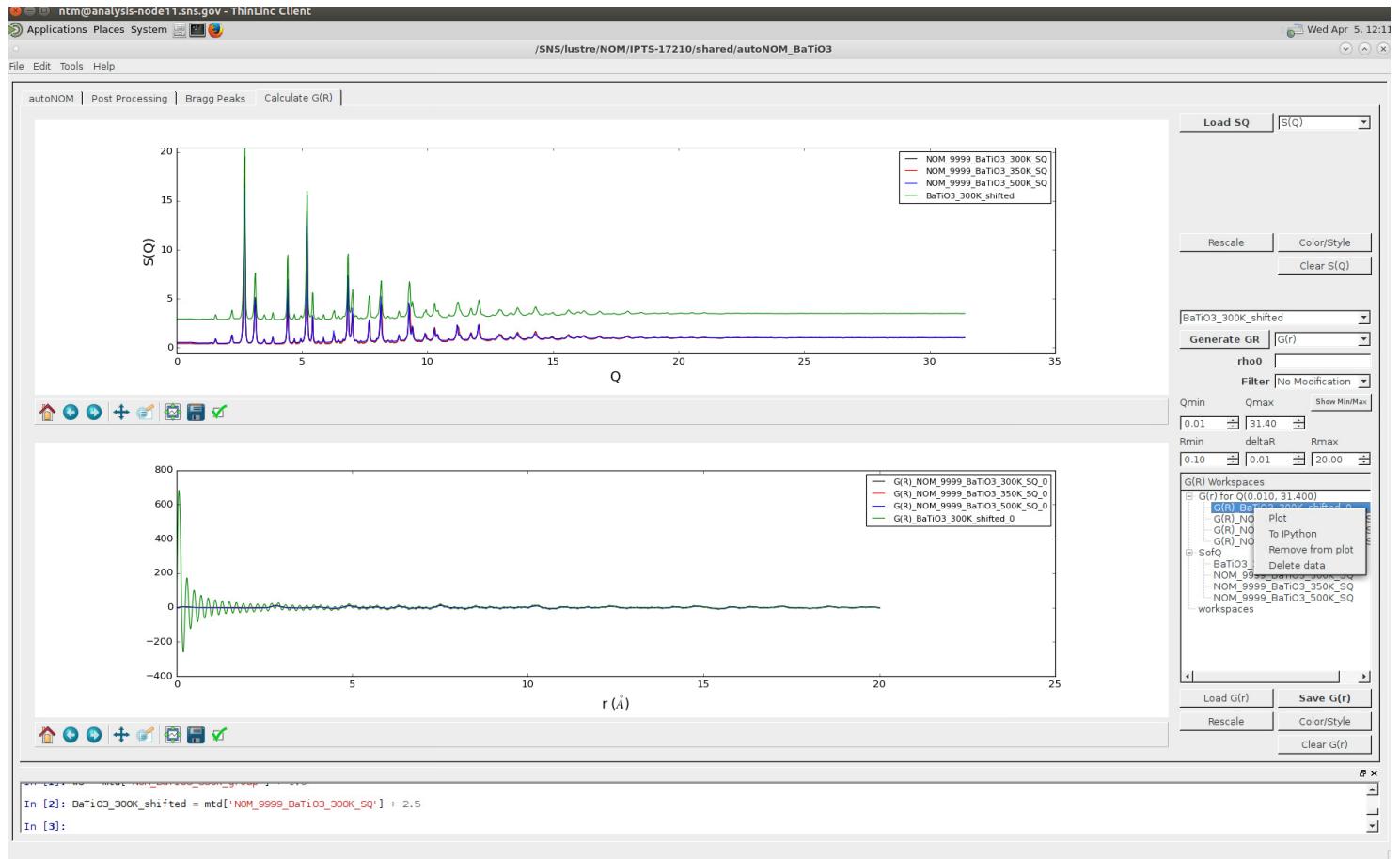
- **Remove from plotting:** Removes dataset from the plot.
- **Delete data:** Deletes the dataset from the **Workspace Tree**.

From the drop-down box above the **Generate G(r)** button, we can select the new S(Q) workspace. Then, we can press the **Generate G(r)** button to perform the Fourier transform on this S(Q) dataset. We see that the new G(r) dataset shows up as a workspace in the **Workspace Tree** under the G(r) subtree. We show an example of this below:

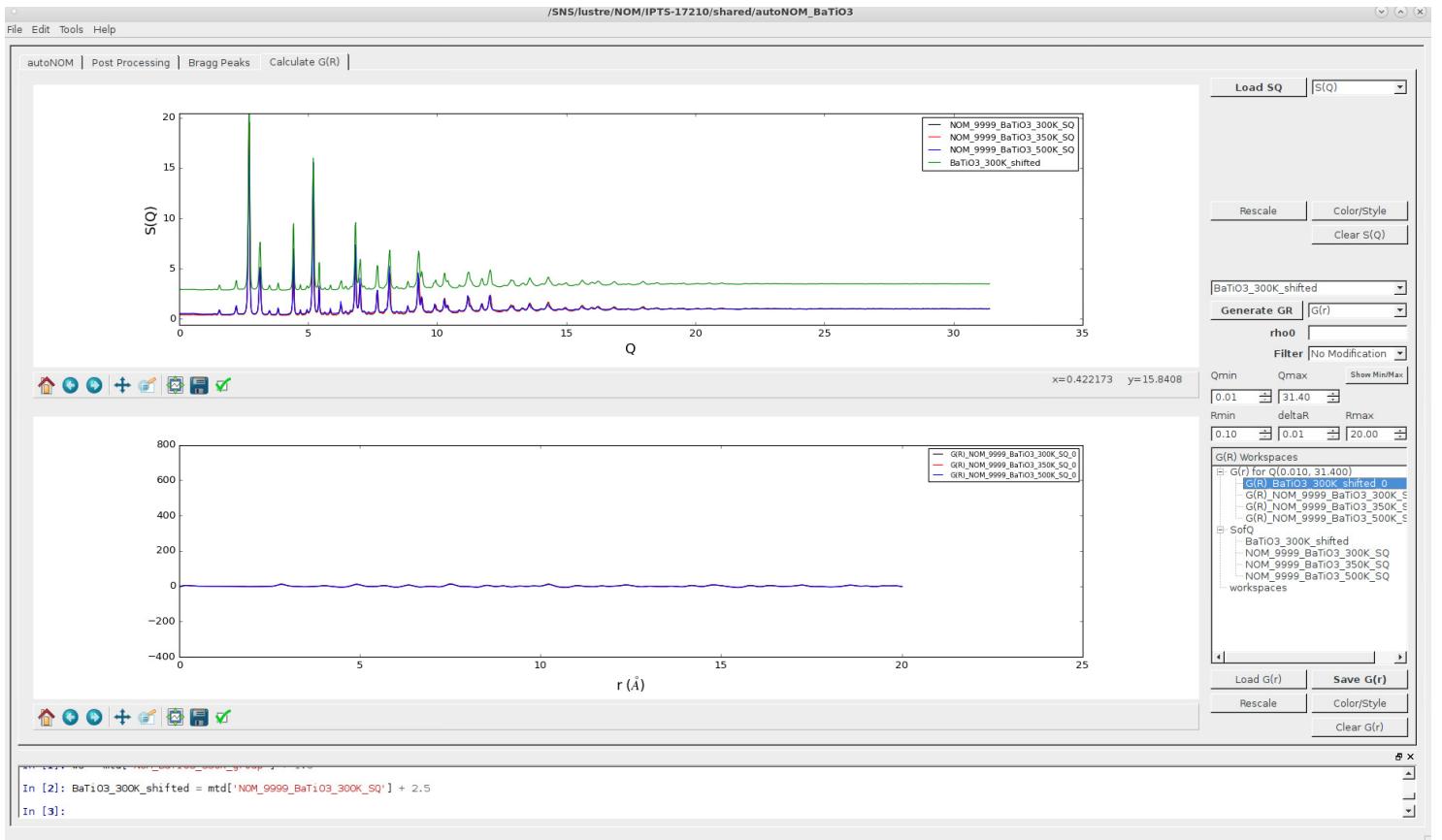


Also, from the drop-down beside the **Generate  $G(r)$**  button, we can also select to generate  $g(r)$  or  $RDF$  (the Radial Distribution Function).

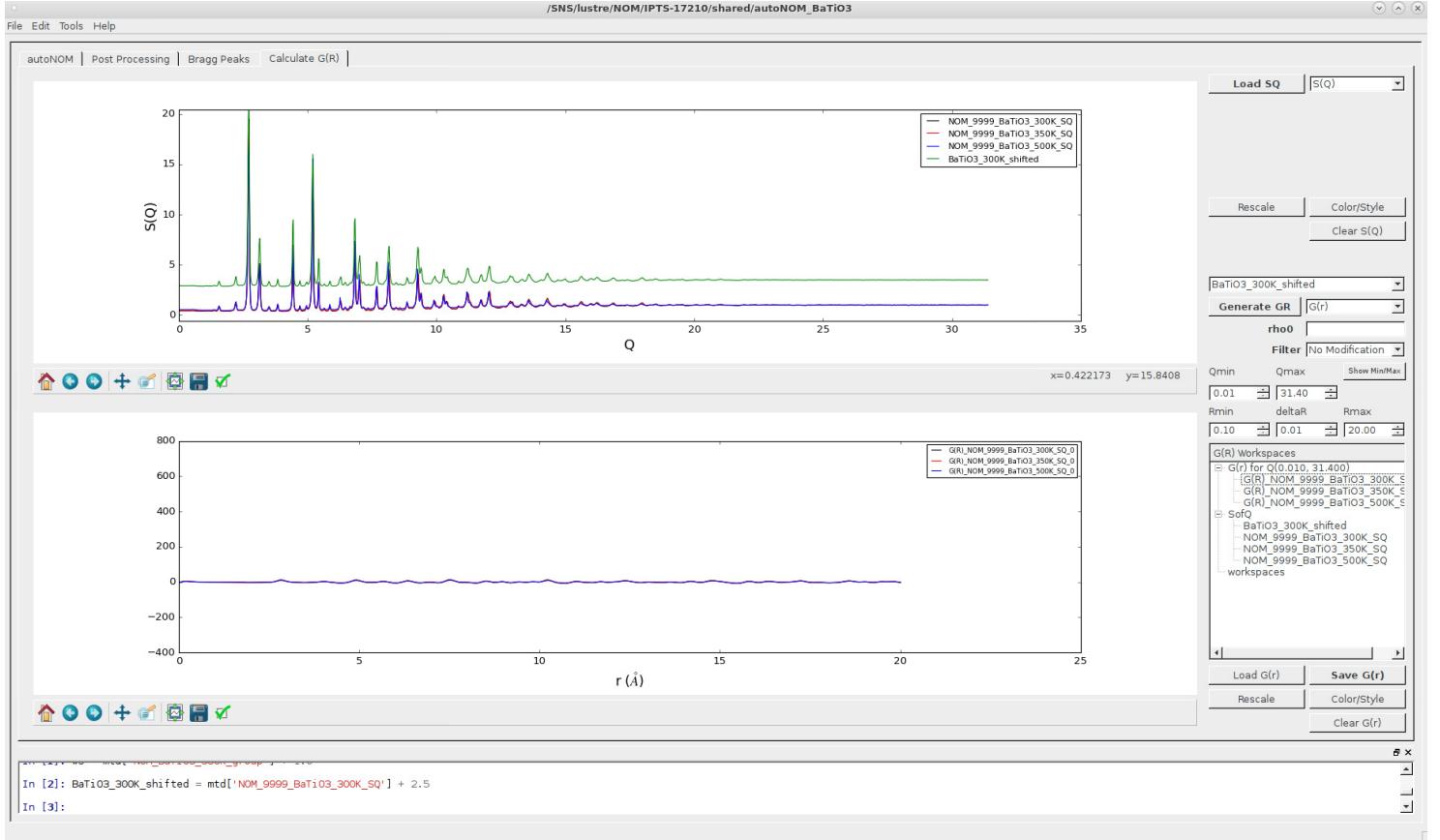
If we right-click, we see that we have the same options for the  $G(r)$  workspaces as for the  $S(Q)$  workspaces:



Below, we have removed the  $G(r)$  workspace that was just created from the plot(the  $G(r)$  **BaTiO3\_300K\_shifted\_0** workspace). Notice, it still exists in the **Workspace Tree**:



Now, we can also delete the  $G(r)$  workspace.. Notice, it no longer exists in the **Workspace Tree**:



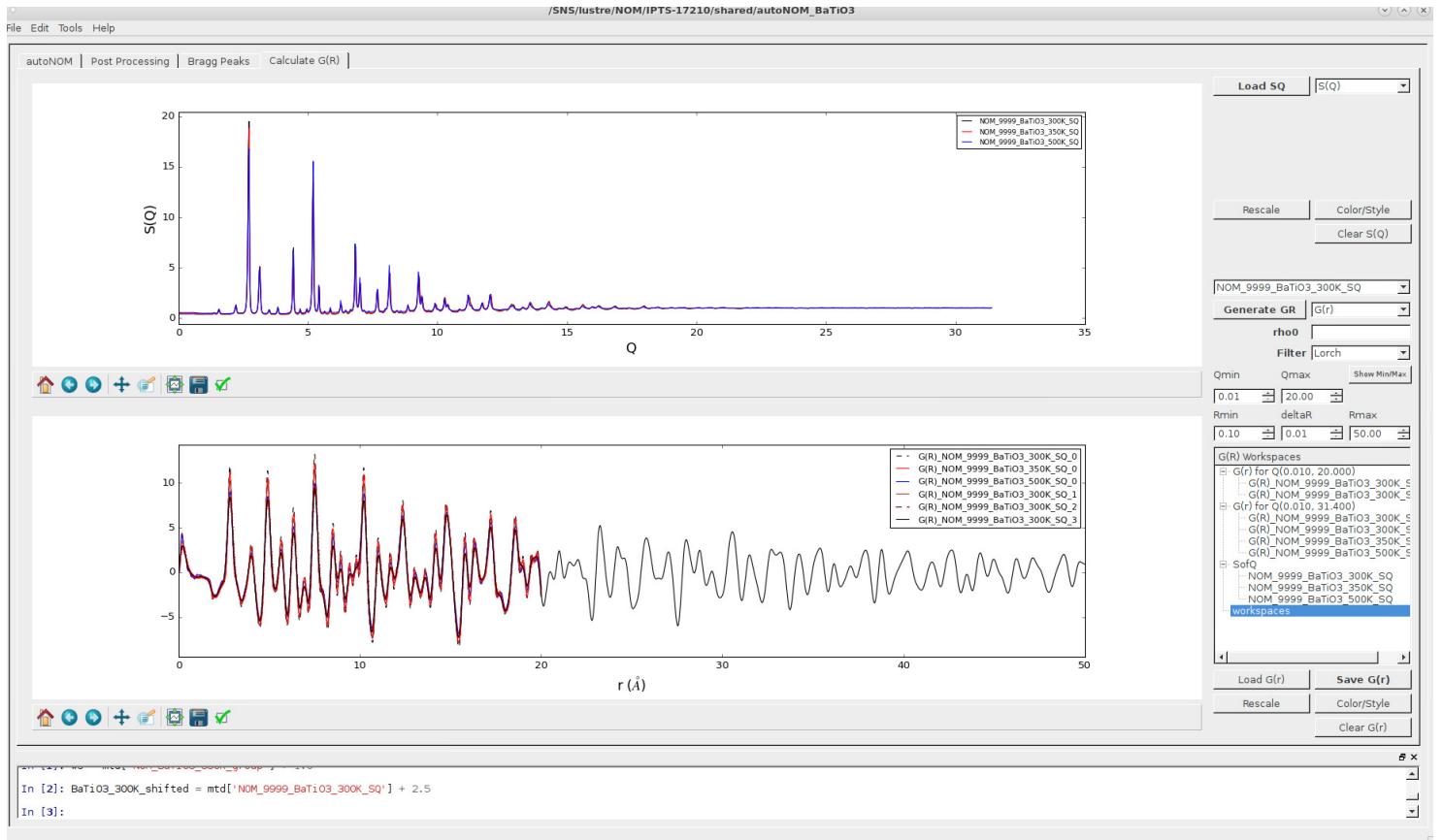
The ***rho0*** field is used to input a bulk density value.

The ***Filter*** drop-down is used to select different function we can use to transform and modify our data. Currently, the options are to apply no such function, **No Modification**, or to use the **Lorch** function. Multiplication with a Lorch function reduced the influence of high  $Q$  noise and leads to smoother  $G(r)$ /PDF data. However, this comes at the expense of real space resolution (multiplication in  $Q$  = convolution in  $r$ ).

The ***Qmin*** and ***Qmax*** specify over what  $Q$  range to perform the Fourier transform to produce a  $G(r)$ . If we press the **Show Min/Max**, we get a visual display in the  $S(Q)$  plot area of these ***Qmin*** and ***Qmax*** values we are using. An example is shown below:



The **Rmin** and **Rmax** specify the minimum and maximum value of the real space data, respectively. The **deltaR** specifies the bin size used for the produced  $G(r)$ . Below, we show where we have extended the Rmax range for the  $G(r)$  produced:



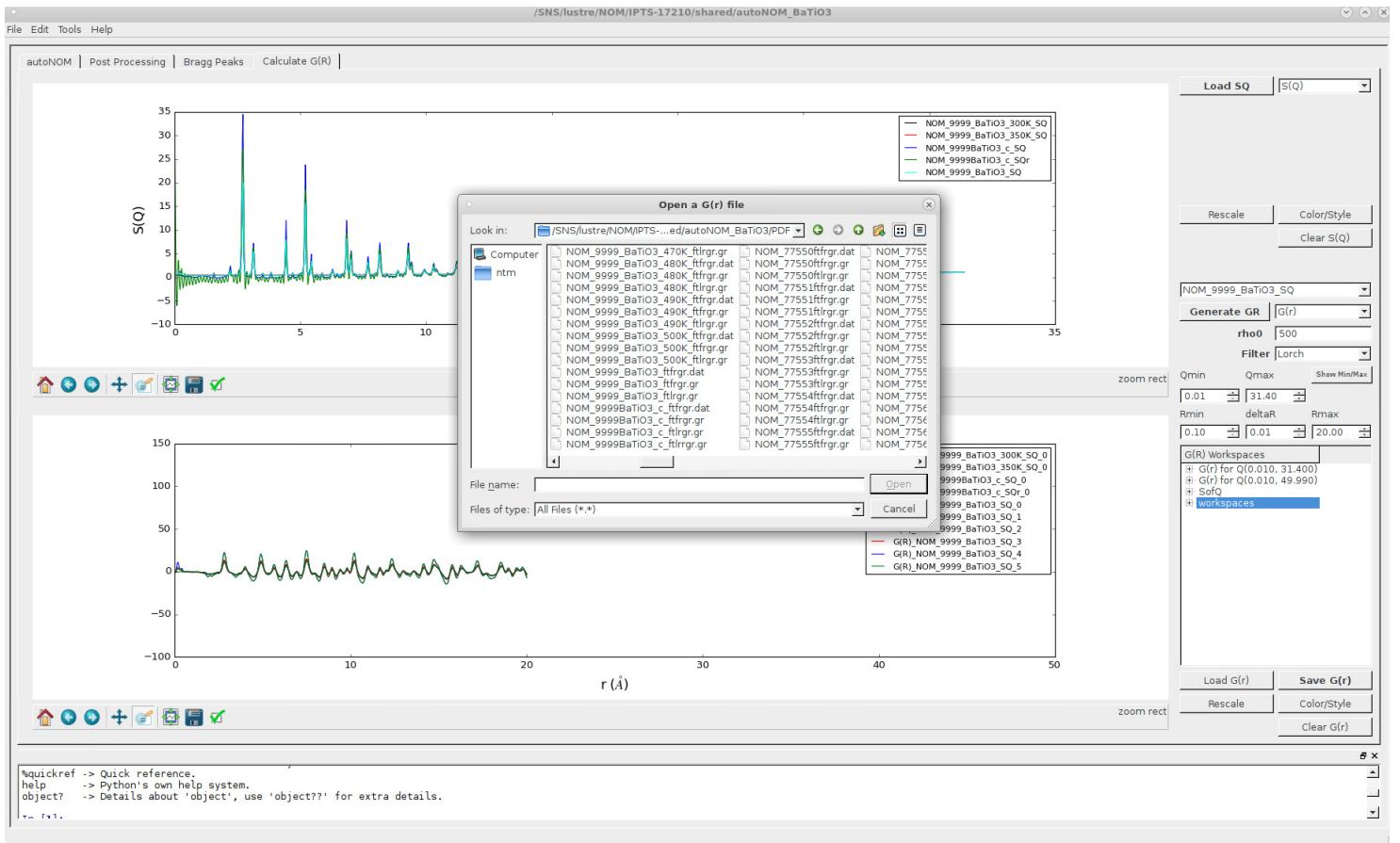
To change the legend, in case it is in the way or masking data, you can right-click inside any of the plot areas and either reduce the font of the text, increase the font of the text, or hide the legend all together. An example is shown below:



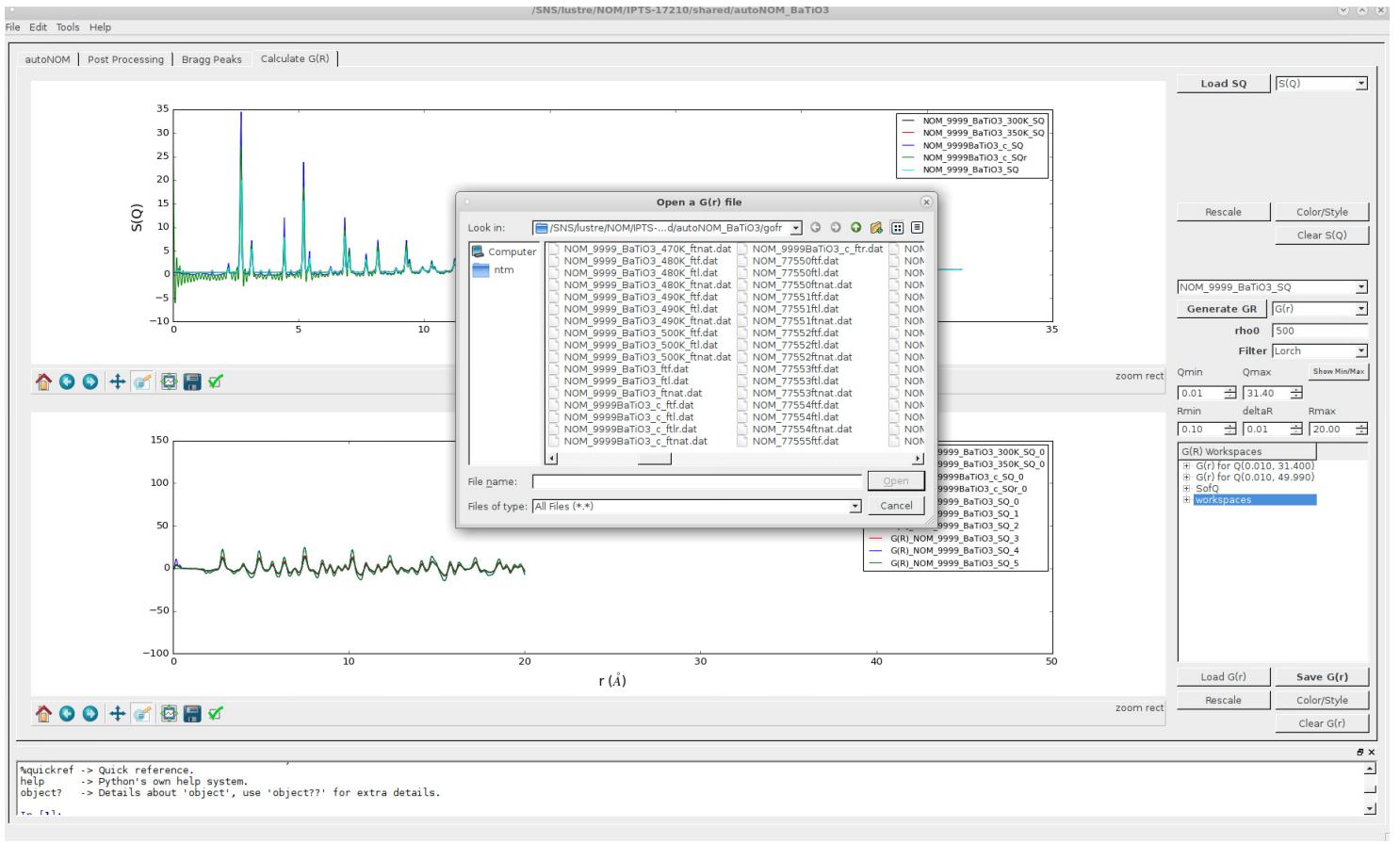
### 4.5.3 Load $G(r)$ data

We can also load in our real space data from the individual runs or post-processed runs that are complete. Go to the bottom right and press the **Load  $G(r)$**  button. You can select either the **gofr** or the PDF file directories.

If you choose the PDF, you should be presented with a file dialog similar to the one below:



If you choose the `gofr`, you should be presented with a file dialog similar to the one below:

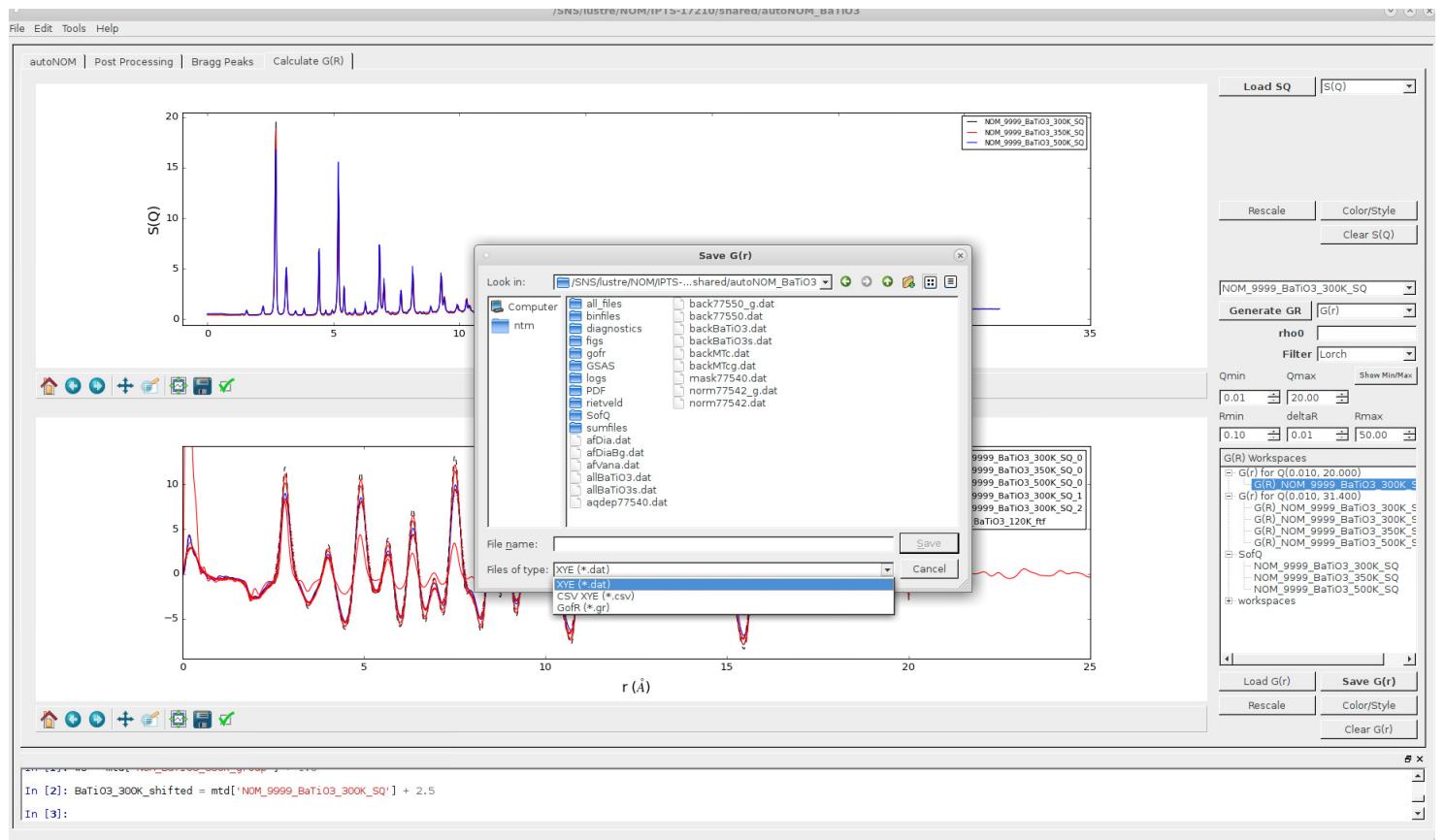


For the different file types of both, we have the following:

- NOMXXXftfrgr.gr – G(r) or PDF of your samples, ready for analysis for PDFgui software package
- NOMXXXftlgr.gr – the same, but convoluted with the Lorch function
- NOMXXXftl.dat, NOMXXXftf.dat – small g(r)

#### 4.5.4 Output G(r)

The **Save G(r)** button will allow you to output your selected G(r) workspace into a variety for file formats. Currently, you can output it to the following formats:



#### 4.5.5 Optimize G(r)

Insert the optimization strategies we have discussed for each instrument scientist's method

**Add references through manual**