Manual for WAND² Powder Data Reduction

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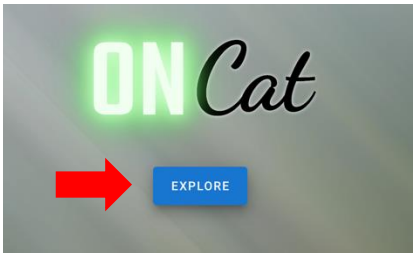
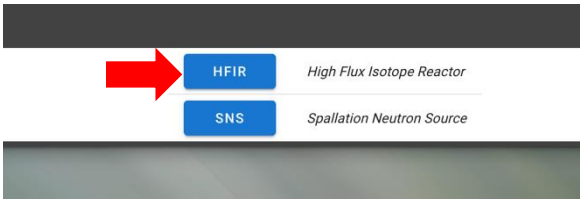
In this manual, you will find detailed instructions on how to load, reduce, and save powder diffraction data using MantidWorkbench Nightly. Instructions on how to use MantidWorkbench Nightly can be found in the dedicated manual (same webpage).

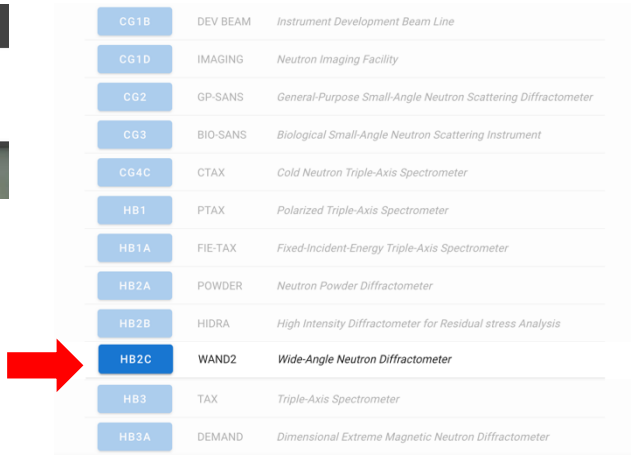
I) Loading data:

1) Go to https://oncat.ornl.gov/#/ to correlate scan numbers to the scan title so you know what scan ranges are relevant for the reduction, and download data for Mantid if necessary. Click “Explore” and log in to OnCAT catalog with UCAMS.

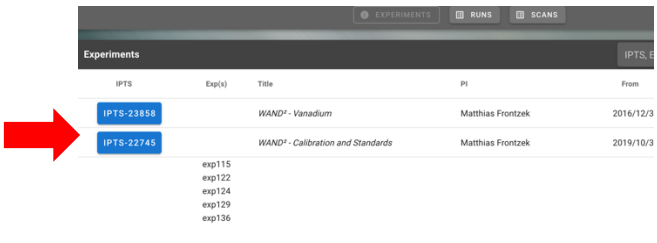


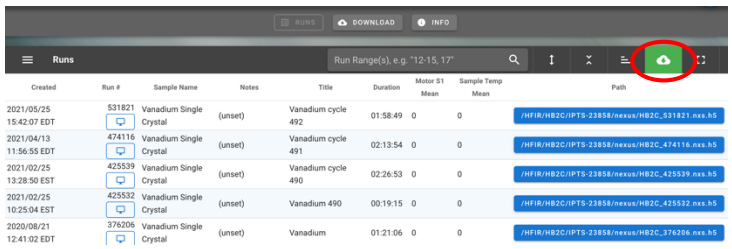
2) Search for proposal number (IPTS) through: HFIR→ HB-2C→ IPTS.





3) Hit the according IPTS and click download icon for a file with data.





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4) Note run numbers for sample and Vanadium normalization found in excel downloaded file. You will need the Vanadium IPTS and scan number to input to the powder reduction algorithm.

2021/05/25 15:42:07 EDT	531821	Vanadium Single Crystal	(unset)	Vanadium cycle 492	01:58:49
2021/04/13 11:56:55 EDT	474116	Vanadium Single Crystal	(unset)	Vanadium cycle 491	02:13:54
2021/02/25 13:28:50 EST	425539	Vanadium Single Crystal	(unset)	Vanadium cycle 490	02:26:53
2021/02/25 10:25:04 EST	425532	Vanadium Single Crystal	(unset)	Vanadium 490	00:19:15
2020/08/21 12:41:02 EDT	376206	Vanadium Single Crystal	(unset)	Vanadium	01:21:06
2020/08/18 13:47:32 EDT	368223	Vanadium Single Crystal	(unset)	Vanadium Cycle 489	01:11:20
2020/07/07 13:53:53 EDT	368221	Vanadium Single Crystal	(unset)	Vana cycle 489	02:59:02

5) Go to SNS Cluster Link at https://analysis.sns.gov/ and log in with UCAMS username and password. You can find more information on how to access ThinLinc client session and how to use MantidWorkbench on our website.

6) Once logged in, on the left upper corner, go to Application→Education→Mantid Workbench Nightly.

7) When MantidWorkbench opens, there will be an option to personalize the setup and tutorial available if needed. If a personalized setup is not necessary, close the "Welcome" window. You should see the following on your screen.

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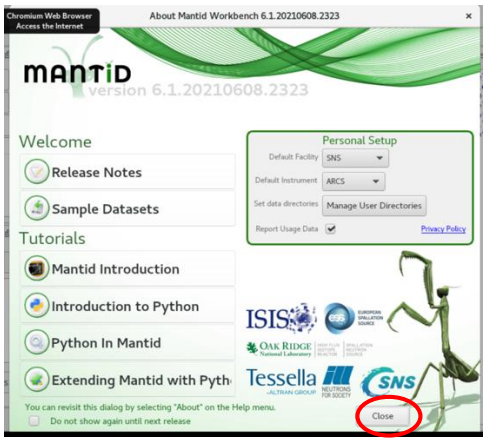
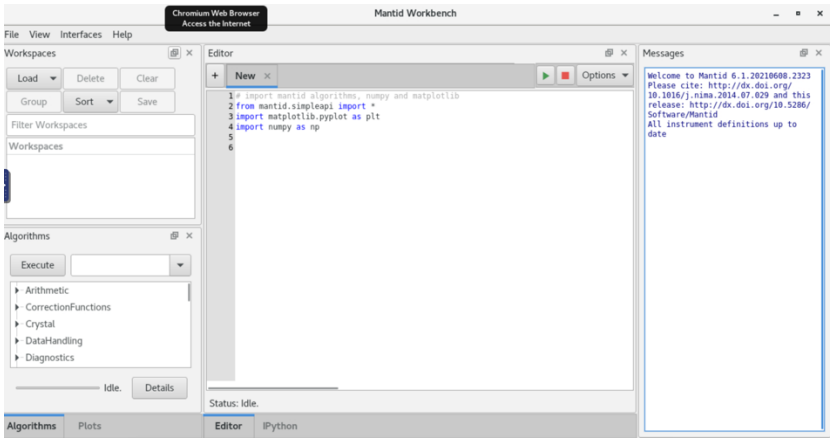
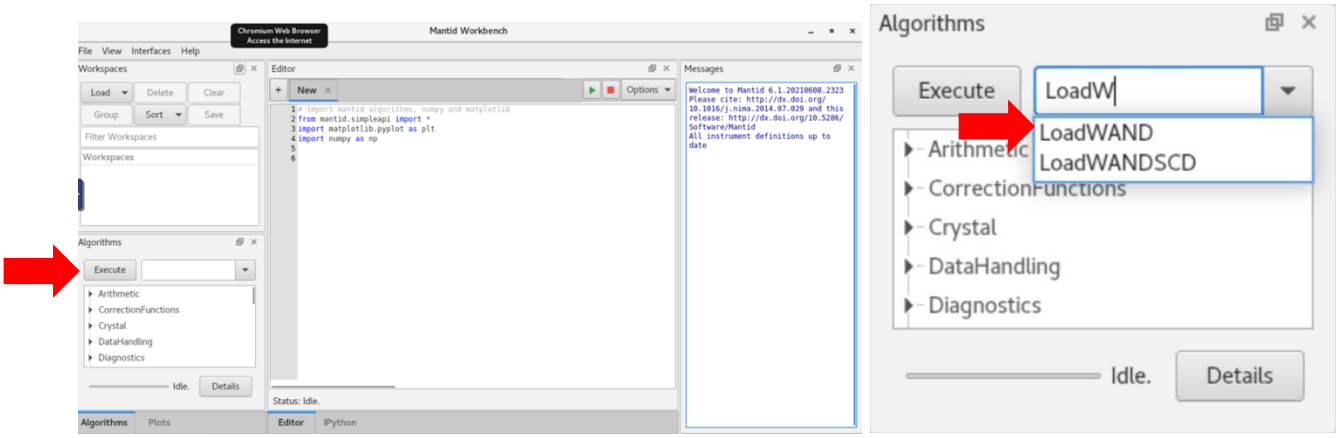
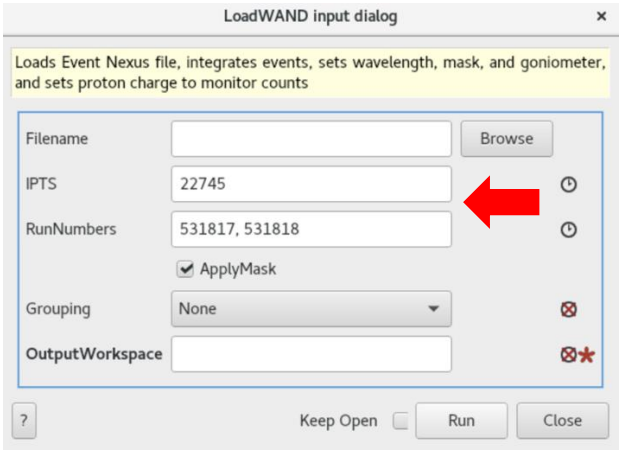




8) Go to Algorithms, and Type "**LoadWAND**" next to 'Execute' for powder data.



9) In the LoadWAND input dialog, enter IPTS and Run Numbers manually (**recommended**) **OR** hit "Browse" to locate IPTS file under data→HFIR→HB2C→According IPTS→nexus; select nexus from IPTS and find run number used.



★ Separate the RunNumbers by comma to load multiple run numbers or use dash to select range.

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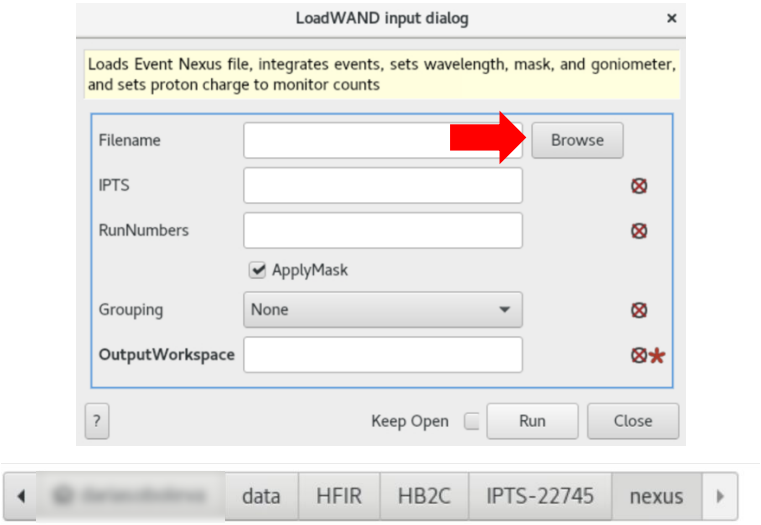
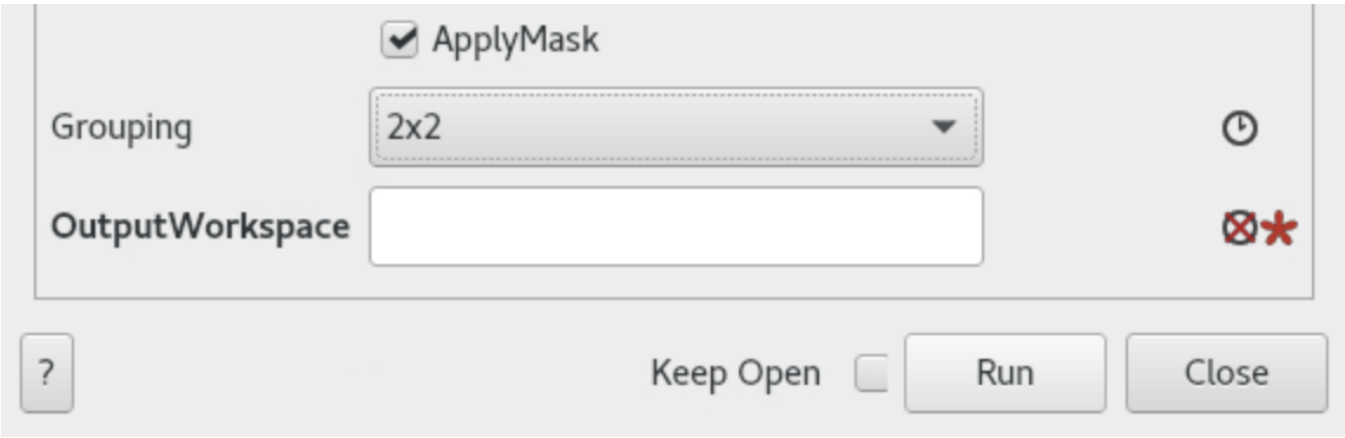
OR



10) Check “Apply Mask” to mask detector edge limits (see algorithm description in docs.mantidproject.org for more information). Use 4x4 grouping if many manipulations will be done with the dataset; use of 2x2 grouping is recommended for faster processing without resolution loss.



11) Name Output Workspace and hit “Run”.

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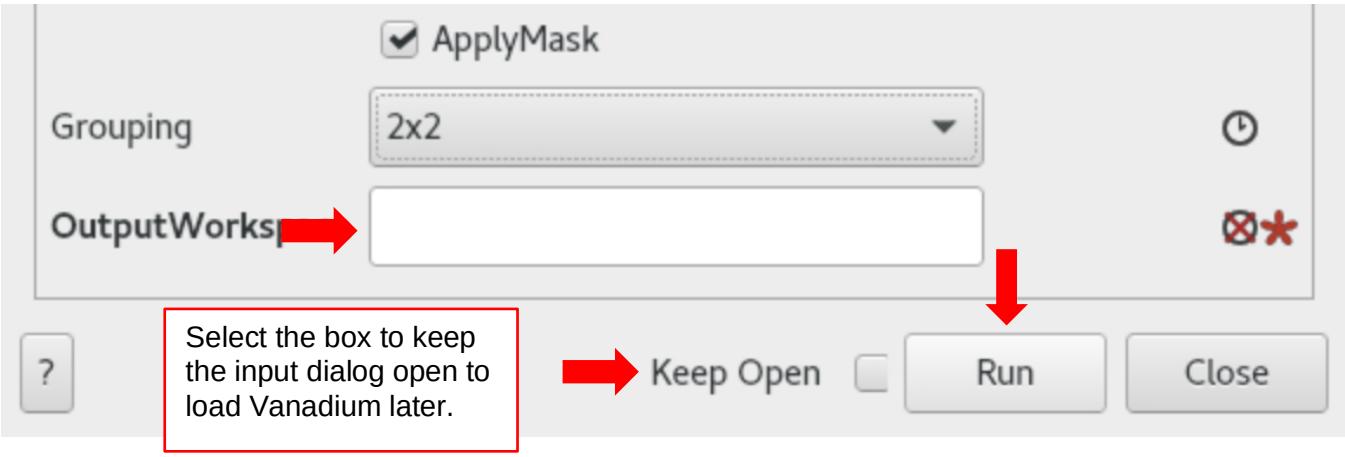
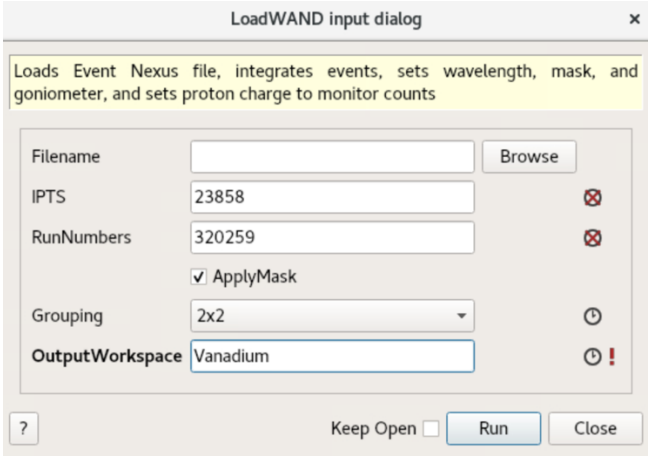
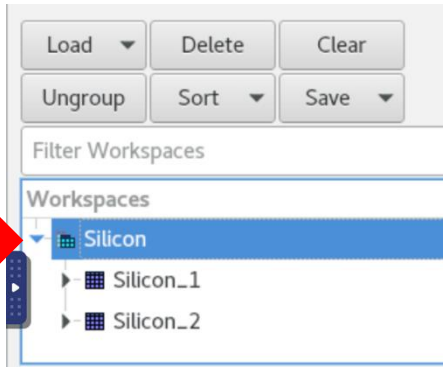


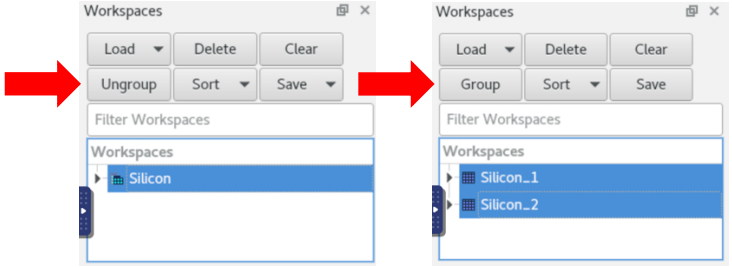
12) To upload Vanadium standard, use Filename or IPTS and run number determined from step 4. Check “Apply mask”, name Output Workspace, and hit run to finish setting up workspace.



13) A folder will be created, which groups all the runs into a single workspace. Click on the arrow to see all the data.



Click on data and select “Ungroup” is necessary. Similarly, select all the data and hit “Group” to reduce two or more files.



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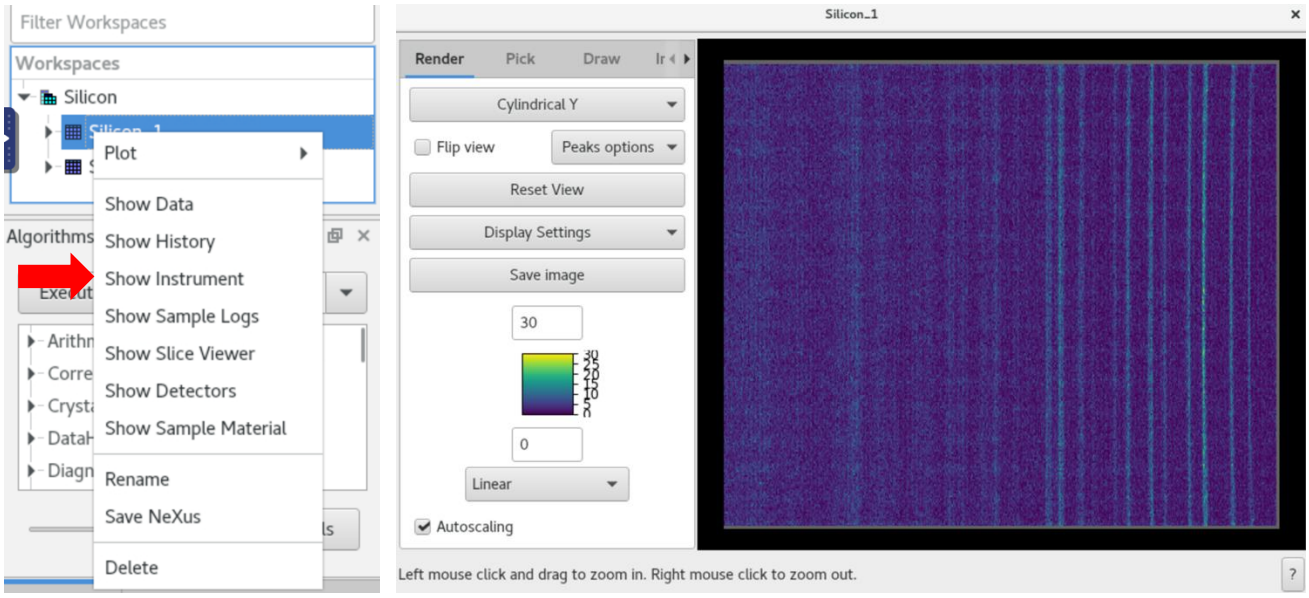
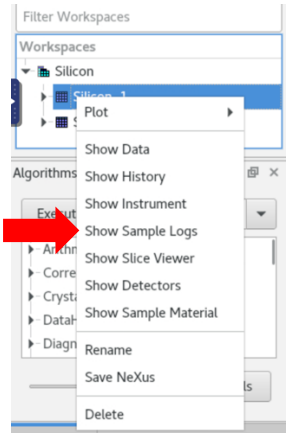
14) To view the data as it was collected on the detector, right click on data file in workspace and click "**Show instrument"**.



15) To view metadata, environmental and instrument parameters for a run, right click on data and select "Show Sample logs" to show values of slits, temperature, and allow them to be plotted to see their values over the course of the run.



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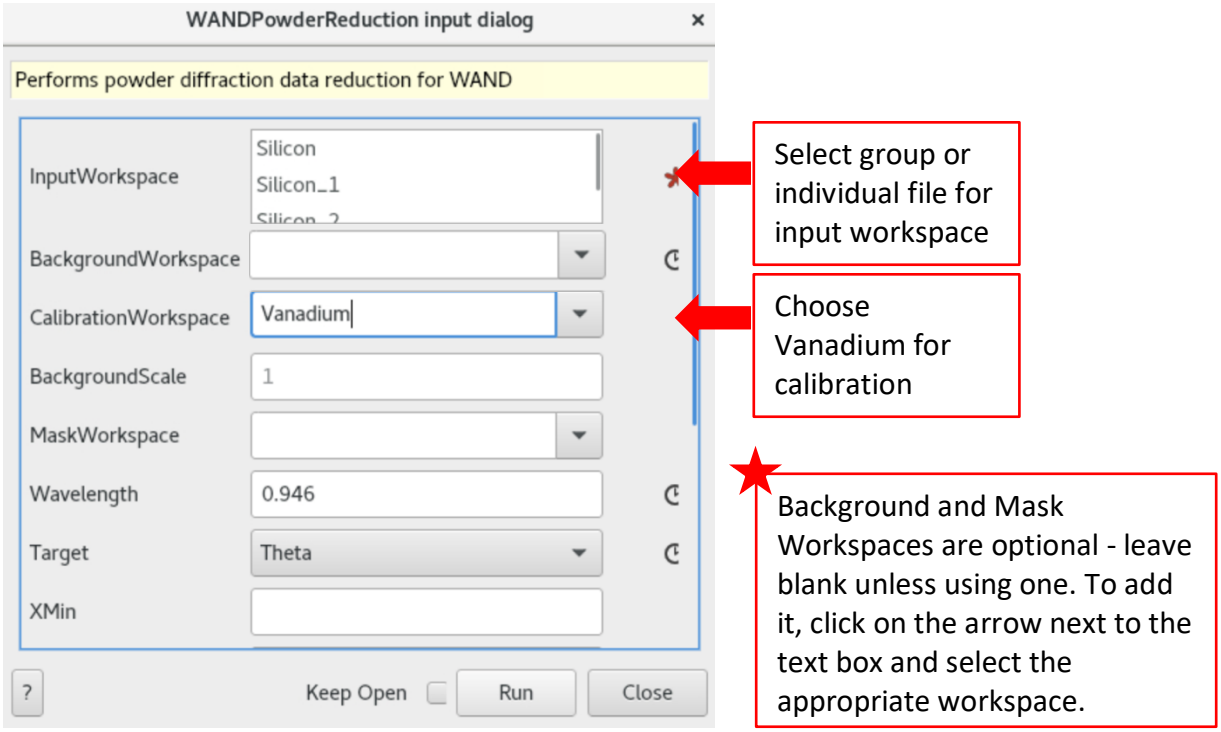
II) Reducing Powder Data:

Now that we've loaded the data into MantidWorkbench, we will integrate it into a 1D powder pattern for use in standard powder analysis software.

1) To reduce the data into a 1D powder pattern, we will use the WANDPowderReduction algorithm. Go to Algorithms, and Type "**WANDPowderReduction**" next to 'Execute' for powder data.

In the WANDPowderReduction GUI, we will need to pick an InputWorkspace (only workspaces loaded prior to the execution of the algorithm will show up in the dropdown list,) a calibration workspace (the Vanadium run,) provide the correct wavelength (usually 1.486AA but could be different depending on your experiment,) the desired x space, bin size and normalization parameters.



2) Scroll down.

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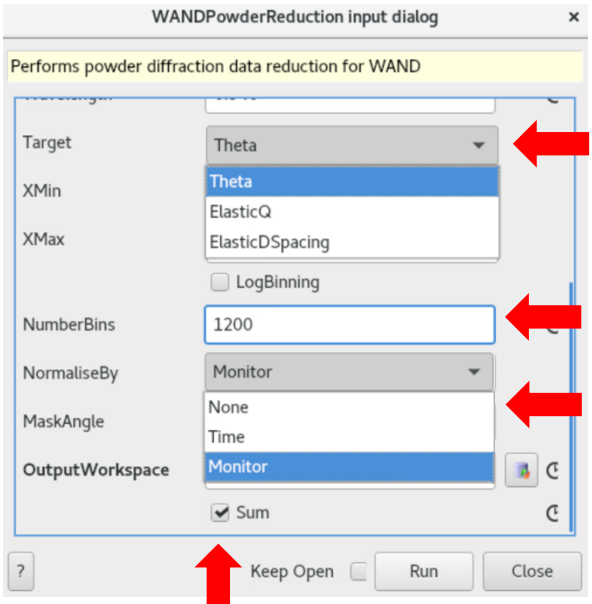


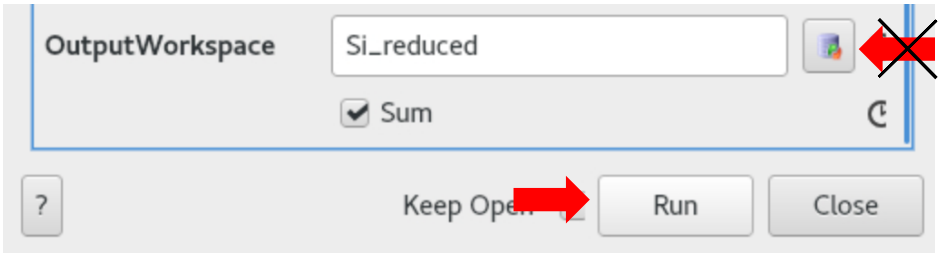
Select "**Theta**" for Target (wavelength not needed if **Theta** is used). If selecting "**ElasticQ**" or "**ElasticDSpacing"** for Target, the wavelength needs to be specified, default value 1.4865 A.

Select value for Number Bins. **1200** is recommended, which does 0.1˚ binning since the detector covers 120˚.

Select "**Monitor**" or "**Time**" to Normalize by; Monitor is recommended, which counts the number of neutrons.

Workspaces can be reduced individually or can be summed together by clicking on **Sum** (e. g. measured at two detector positions).

3) Name the Output Workspace and hit "Run". Using the icon on the right will copy calibration workspace name and will not copy the name of the input workspace, so it is not recommended as it can possible overwrite calibration workspace. Name workspaces independently for changes to be made later without reloading the data.



4) After the reduction is completed, right click on the data and select "**Plot…**", then "**Spectrum with errors**" to view reduced powder data and to make comparisons between intensities at different temperatures more meaningful.

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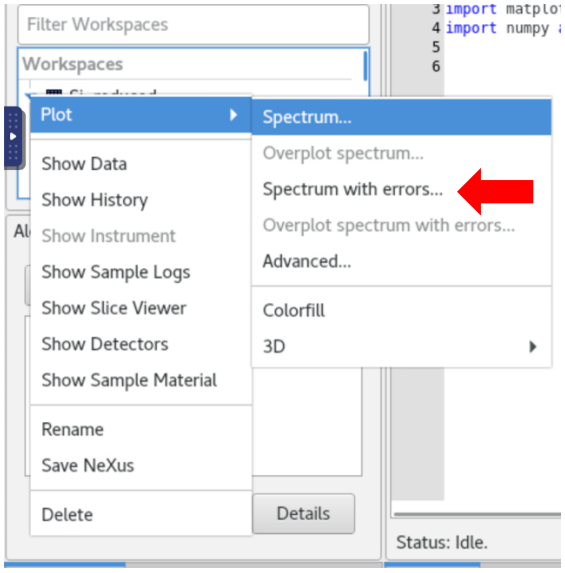
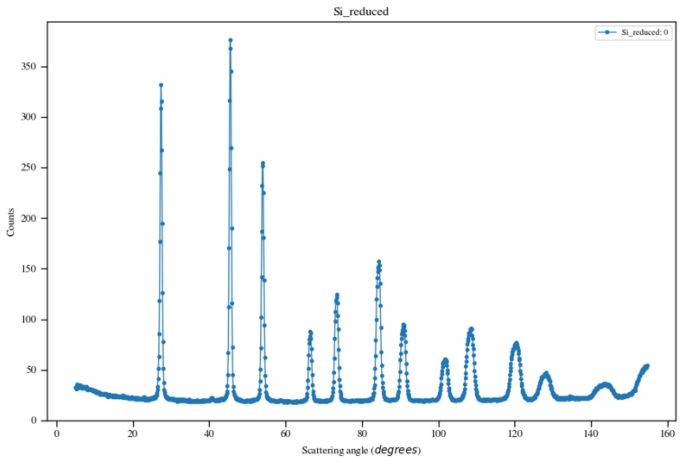
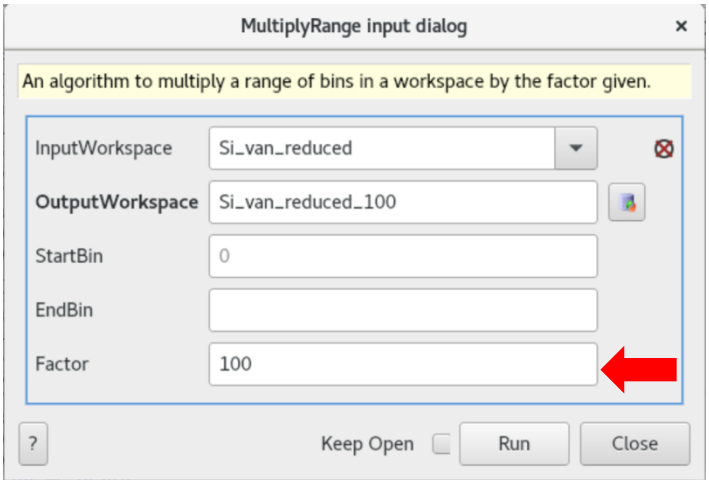




5) Scale data to make it easier for *Fullprof*. Data files have intensities around 1 because they are normalized by the Vanadium. Go to Algorithms and execute "**MultiplyRange**".



Change the factor from 1 to 100. **100** is recommended (though the specific value is not hugely important: it has to be >>1 and be used consistently for all data reduced as part of the same analysis). Hit **Run**.

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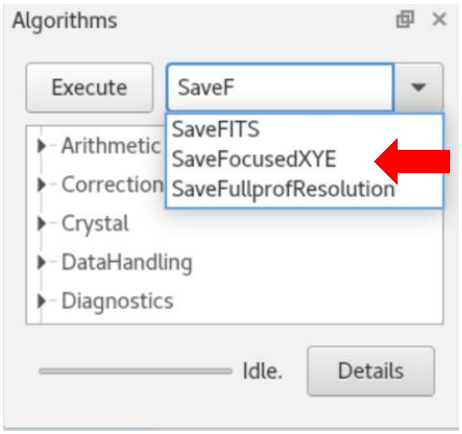
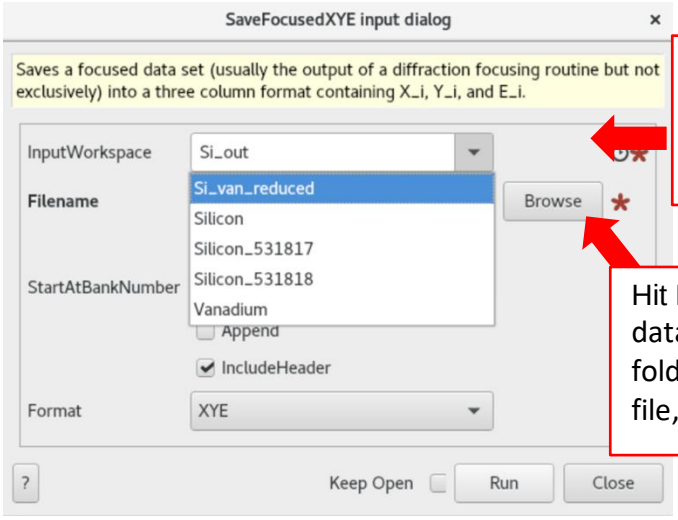
III) Saving Single and Multiple Powder Patterns:

1) Export XYE file in 1 of 2 ways:

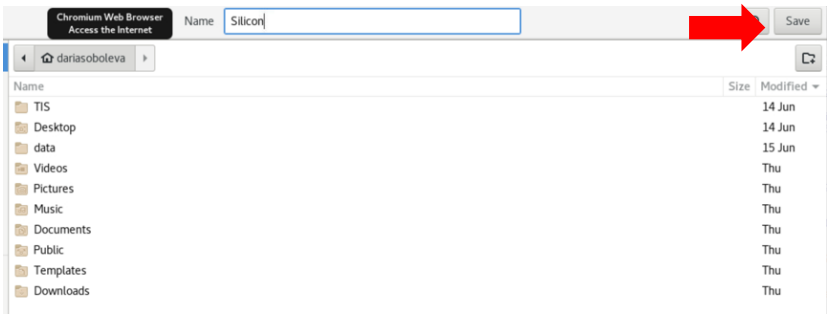
a. When saving one file, execute "**SaveFocusedXYE**".

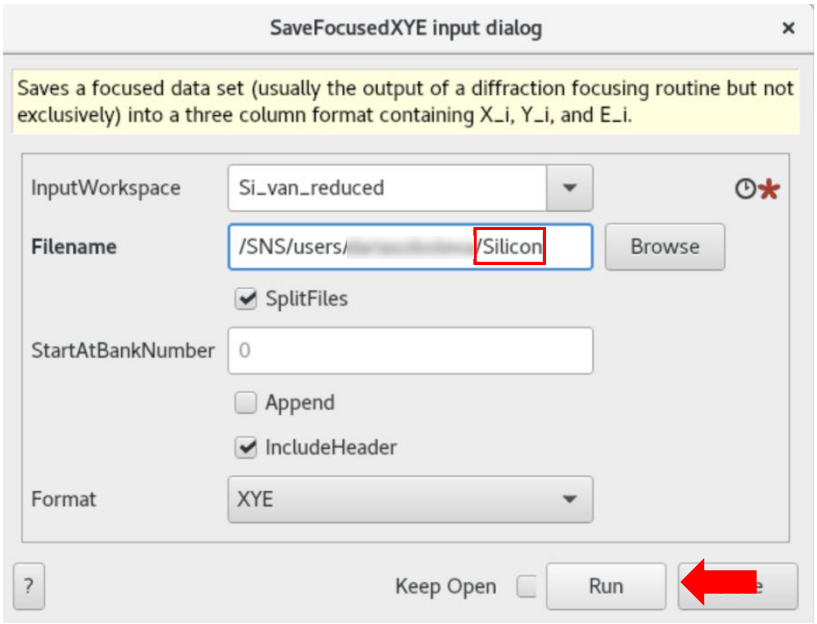




Choose the reduced data for the Input Workspace.

Hit **Browse** to save data in users SNS folder; name the file, hit Save





Hit Run. Then check is the file can be found at the correct place.

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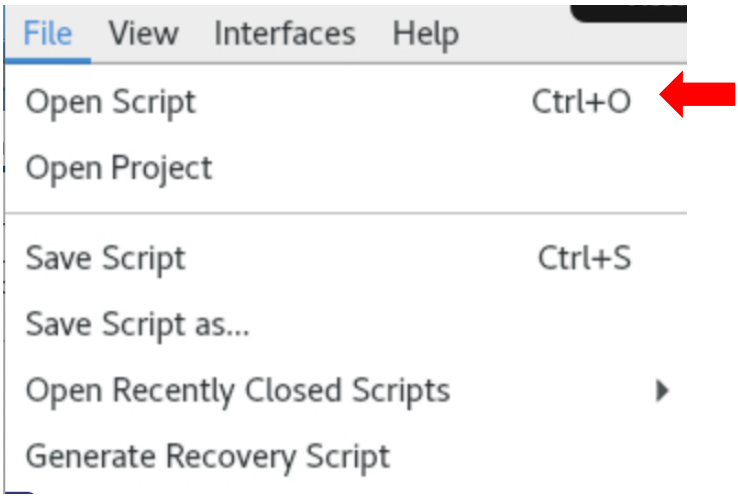
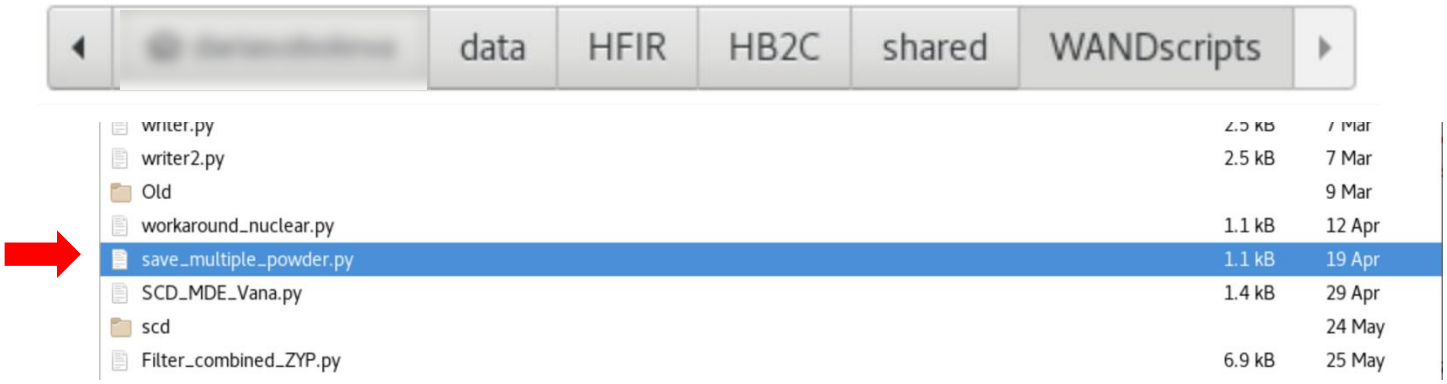
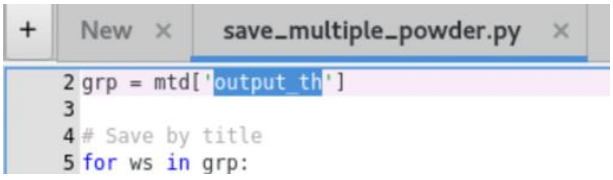
b. When saving multiple powder patterns, make sure that the files are grouped. Once they are, go to **File** on the left upper corner and hit "**Open Script**" or **Ctrl+O.**

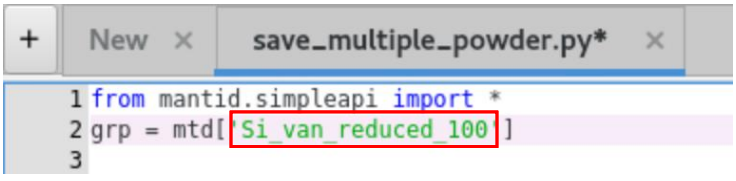


i. Follow the path data→HFIR→HB2C→shared→WANDscripts and locate "**save_multiple_powder.py**".



ii. Before running the script, it is necessary to change the group workspace name to the one used in your reduction and then select the code snippet for how you wish to name the saved the individual files Edit file by editing the second line, group name. Type output workspace into brackets.





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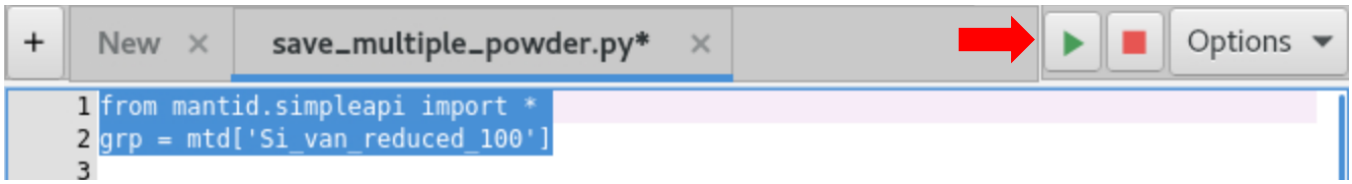
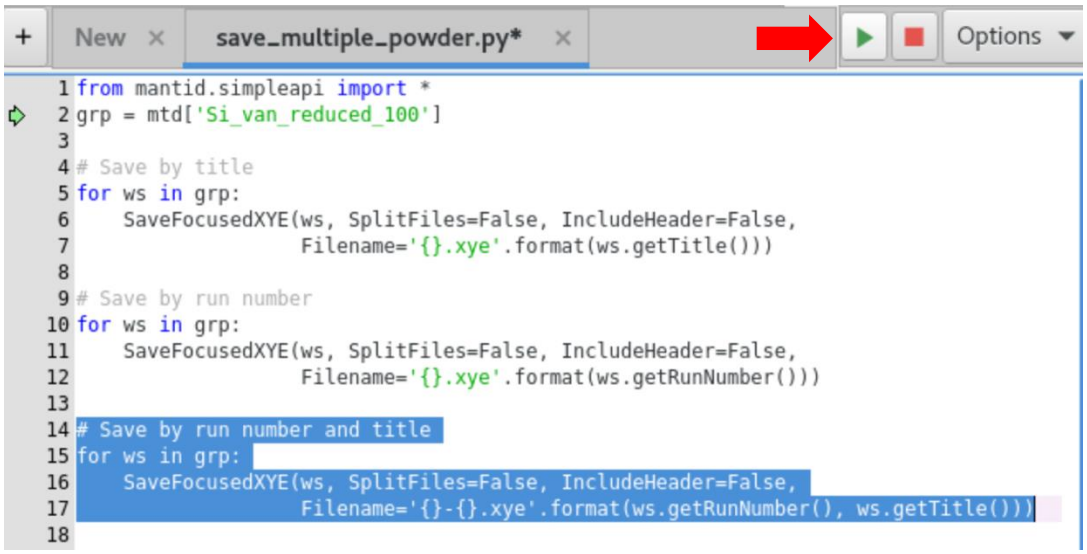
iii. Highlight the first two lines of the script (or hit **Ctrl + Enter**) and hit Execute. Running these two lines will load into mantid a variable with the name of the workspace you want to save.



iv. Next, you will have to decide how you wish to name the saved files and select the relevant code snippet for that naming convention. The script has several options, to save by run number/title, by run number, by run title, by time averaged value, etc. Highlight the **#Save by run number and title** and all the lines below to save the file by title and run number; similarly, the file can be saved by other characteristics (**#Save by run number** the **#Save by title, #Save by time average value,** etc.). Once you've highlighted the relevant code snippet click run (or **Ctrl + Enter**) to execute those lines of code.



v. In order to locate the saved data, go to File, navigate to the folder where you've been saving the files, and click on Modified to organize by the latest modification.

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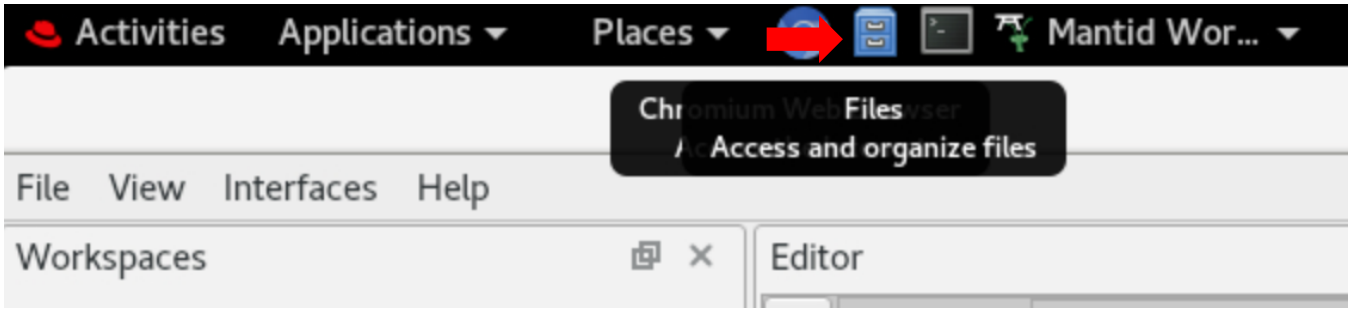

vi. If you want to download these files for use with Rietveld refinements on your local PC/laptop, you can either use a server storage service like Google drive or Dropbox, or download using FileZilla or WinSCP (link on the webpage)..

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