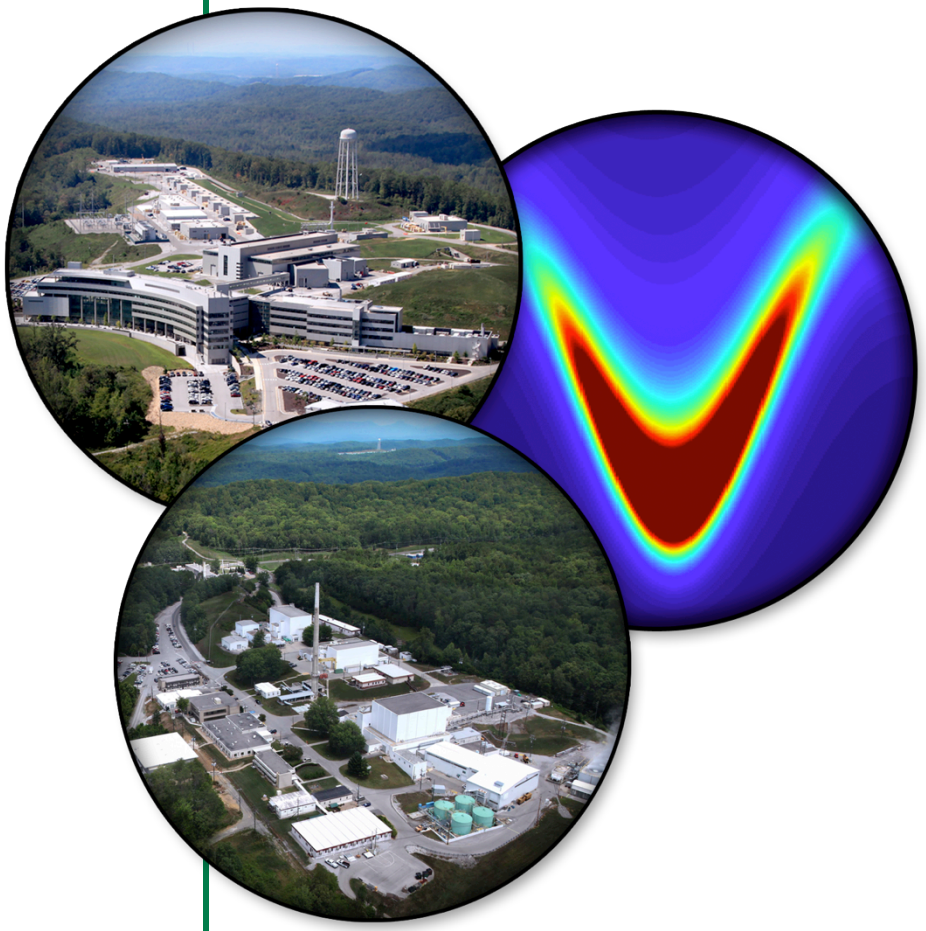
REDUCING HB2A DATA INTO FULLPROF OR GSAS FILE FORMAT



HB2a Instrument Team

July 2014

U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

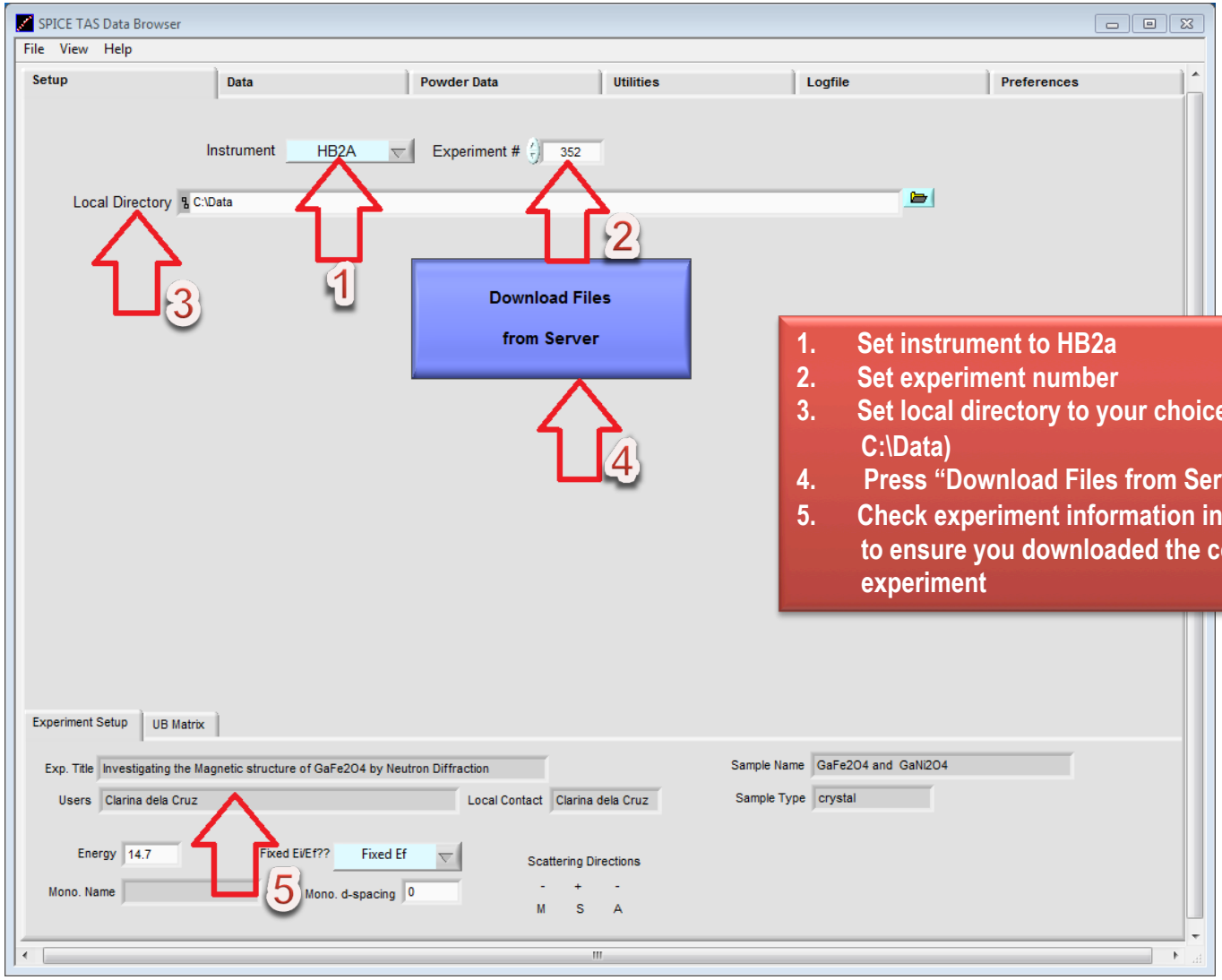
Access to HB2a DATA

- The Hb2a experimental files are accessible on the instrument using the running SPICE data acquisition and data reduction system
- The data may be accessed and reduced remotely by downloading the files from a secure HFIR server using the HFIR Graffiti software which may be downloaded and installed from:

http://neutron.ornl.gov/spice/ or

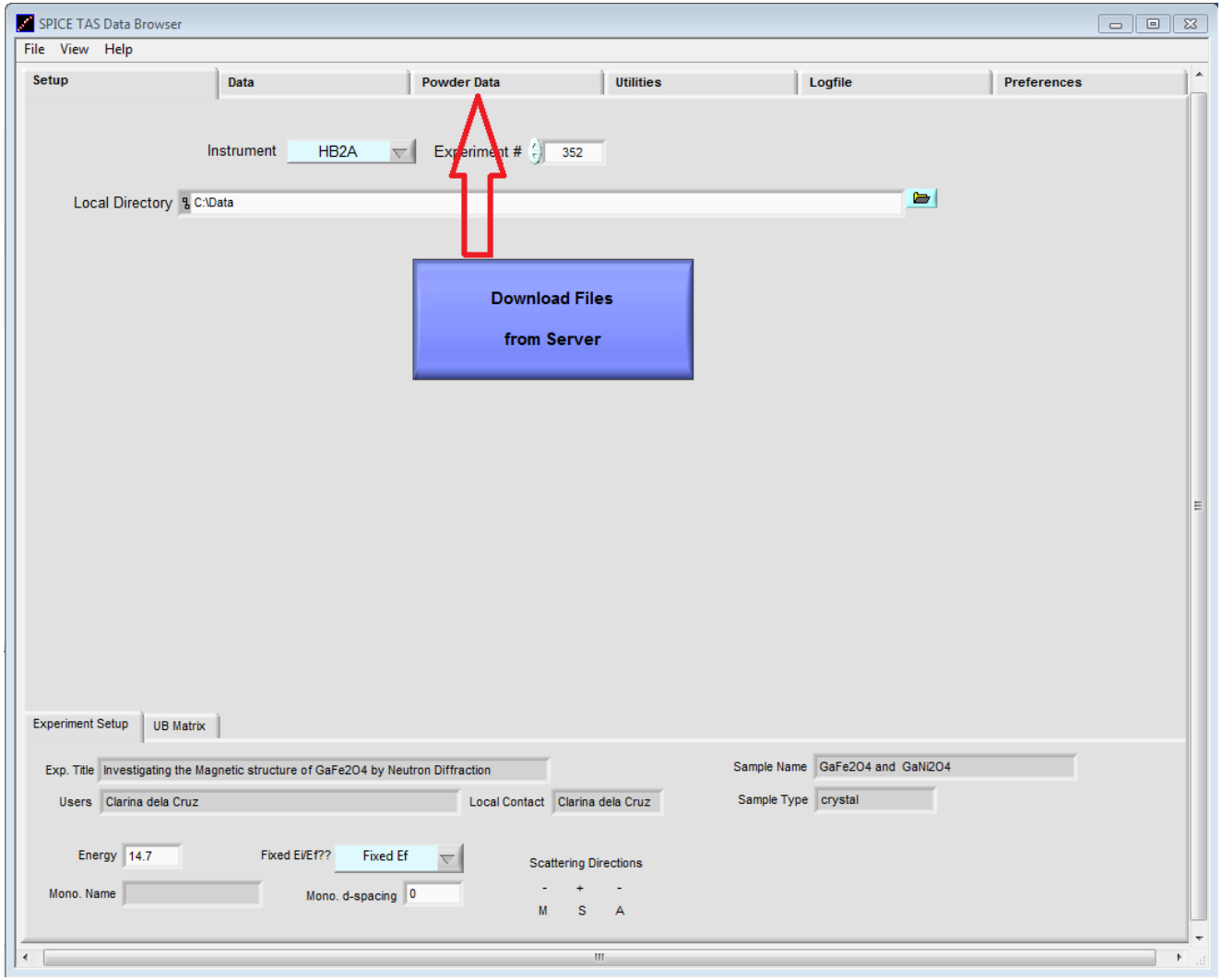
http://neutron.ornl.gov/spice/Executables/GraffitiInstaller%20version%202.6.0.53.exe

If using Graffiti, download the data from server

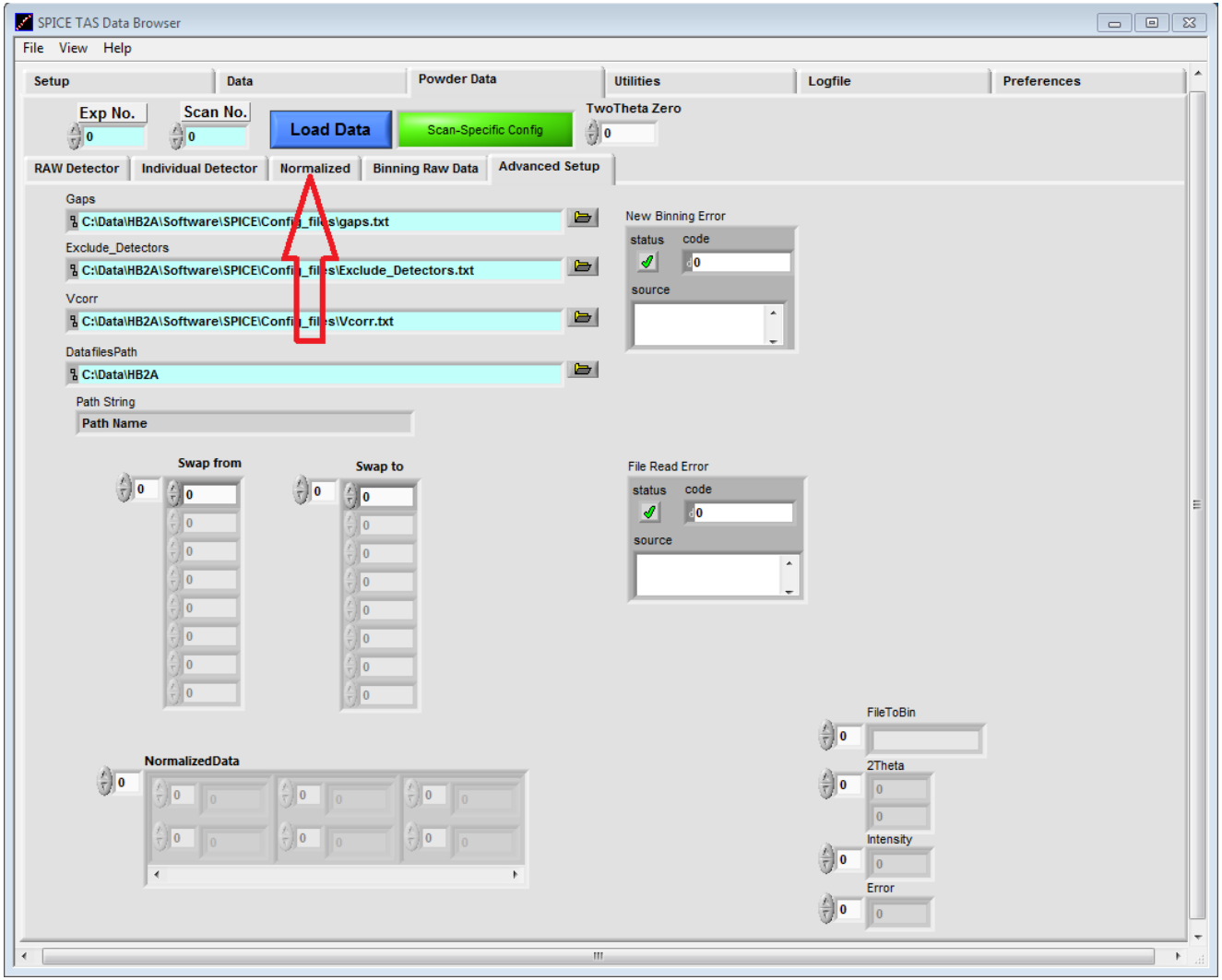


1. Set instrument to HB2a
2. Set experiment number
3. Set local directory to your choice (default to C:\Data)
4. Press "Download Files from Server"
5. Check experiment information in lower part to ensure you downloaded the correct experiment

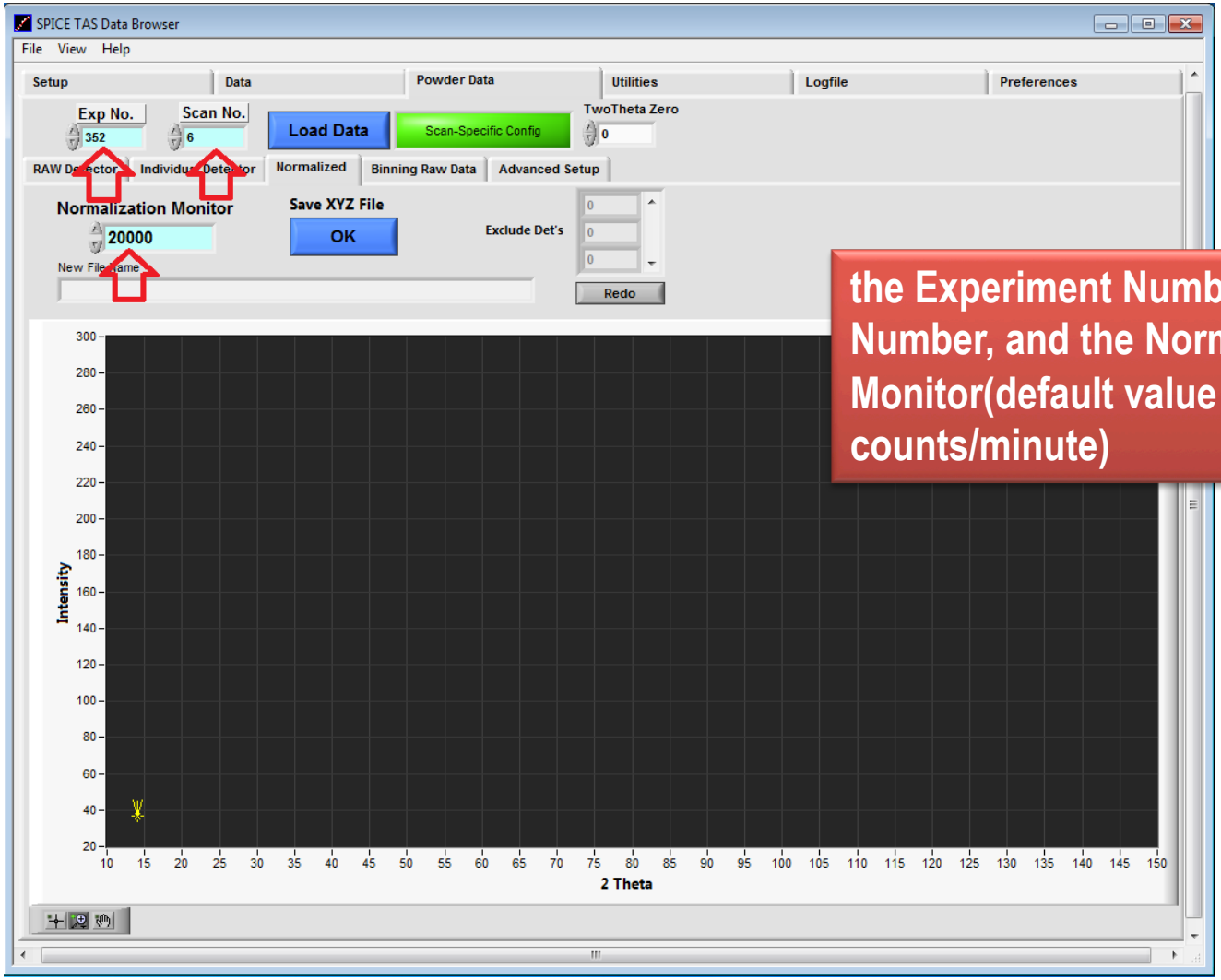
1. Enter the "Powder Data" Tab



2. Enter the "Normalized" Sub-Tab

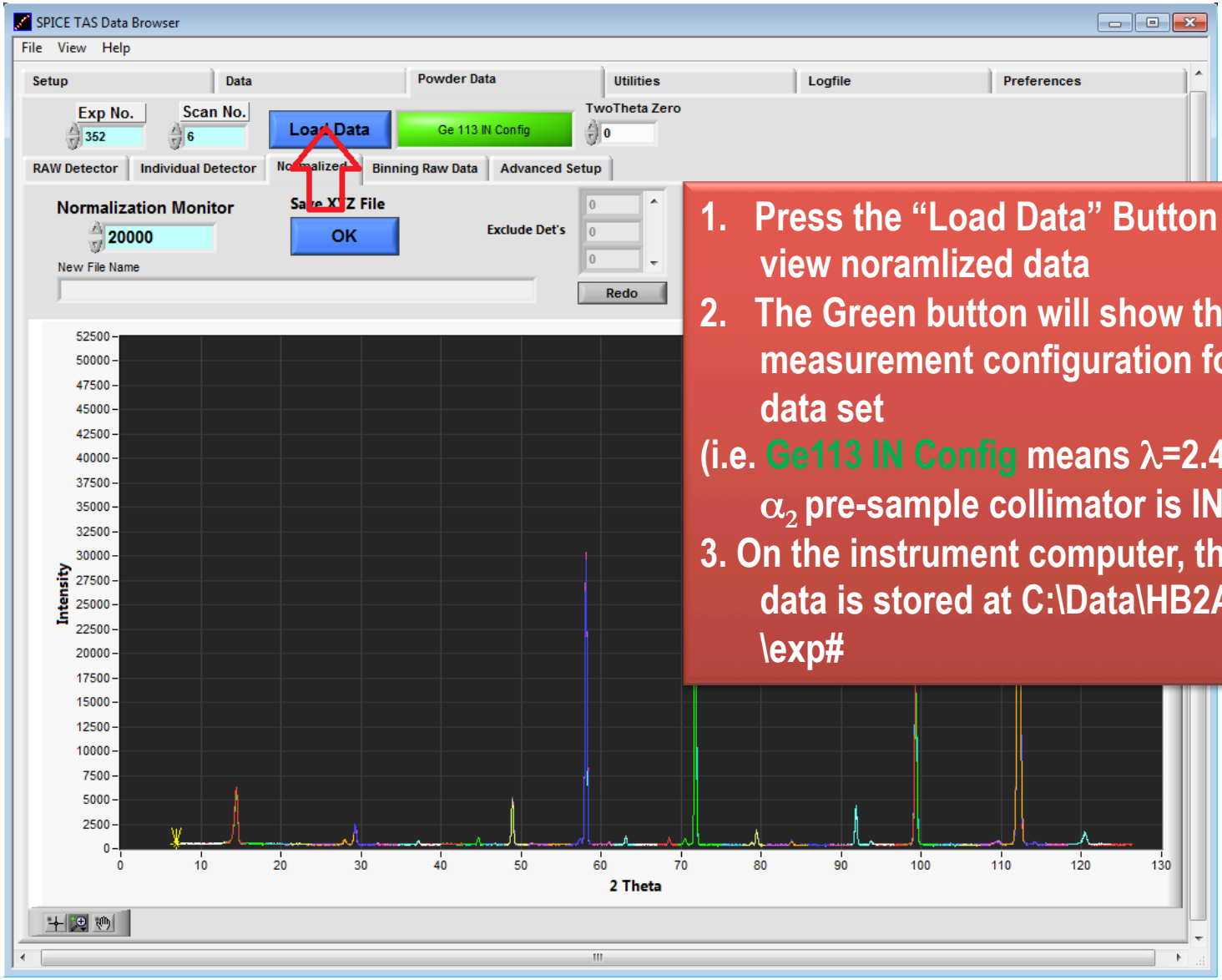


3. Enter data details



the Experiment Number, Scan Number, and the Normalization Monitor(default value at 20,000 counts/minute)

4. Viewing multidetector pattern

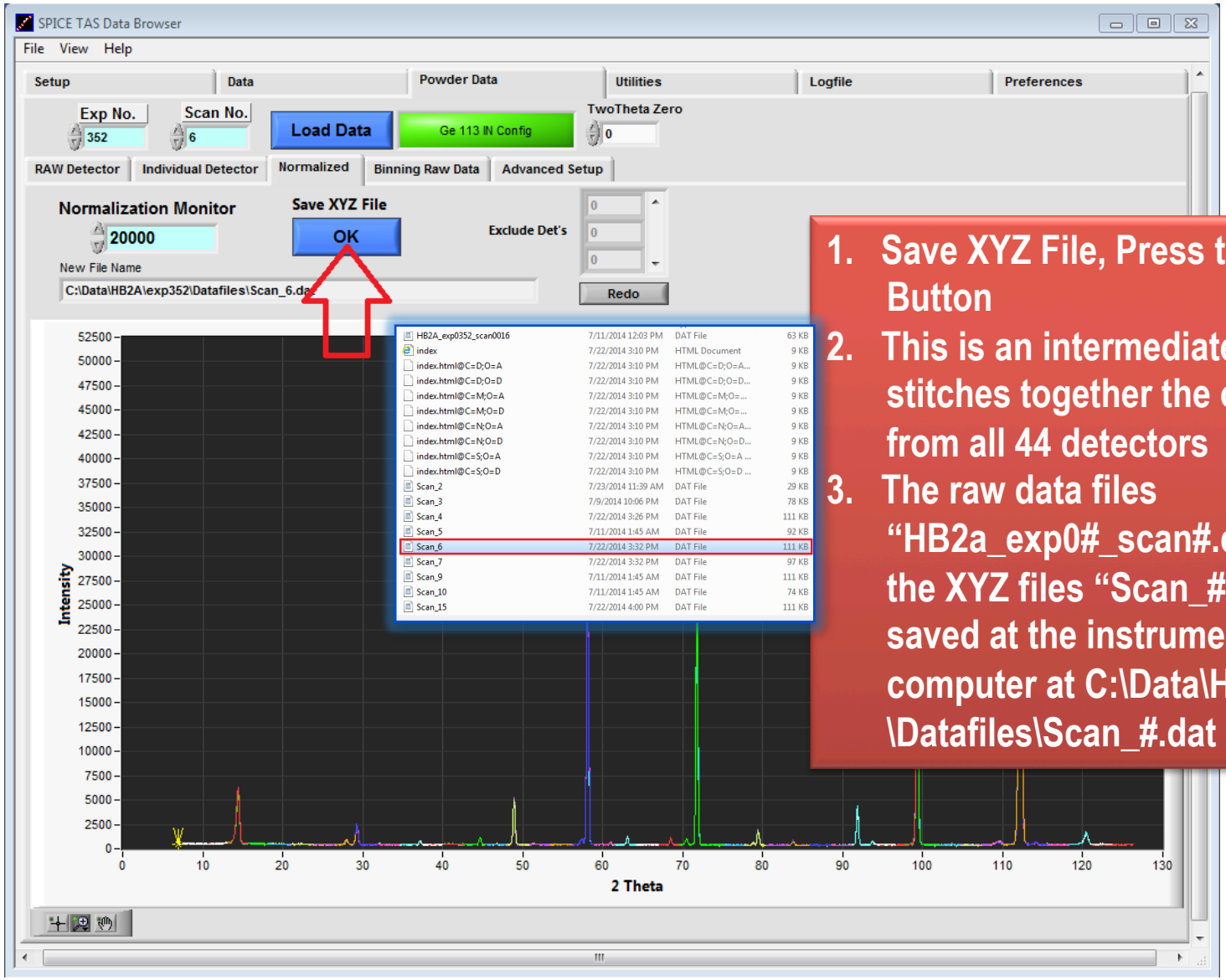


1. Press the "Load Data" Button to view noramlized data
2. The Green button will show the measurement configuration for the data set

(i.e. Ge113 IN Config means λ=2.41Å, α_2 pre-sample collimator is IN)

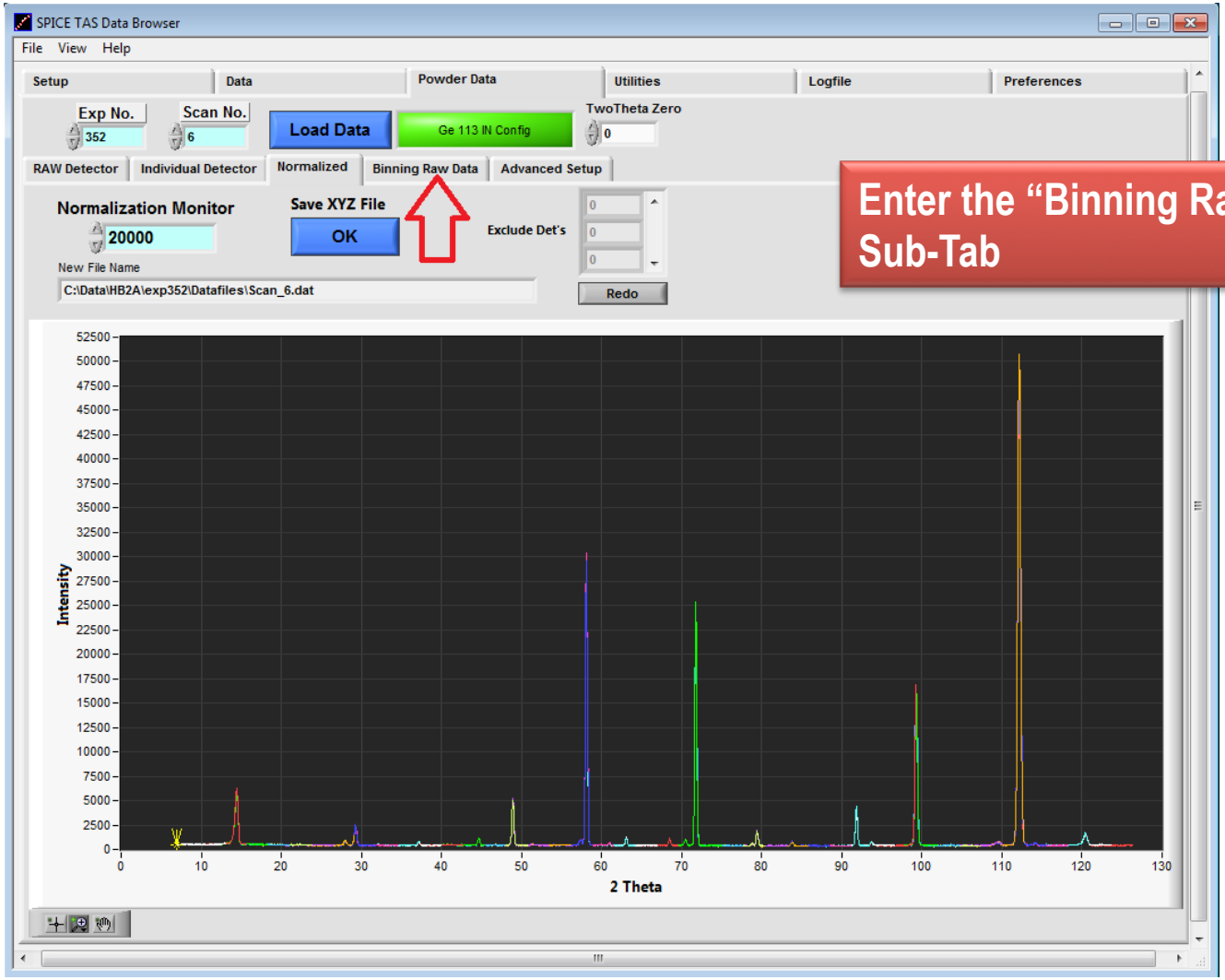
3. On the instrument computer, the data is stored at C:\Data\HB2A \exp#

5. Save 3-column (XYZ) intermediate file



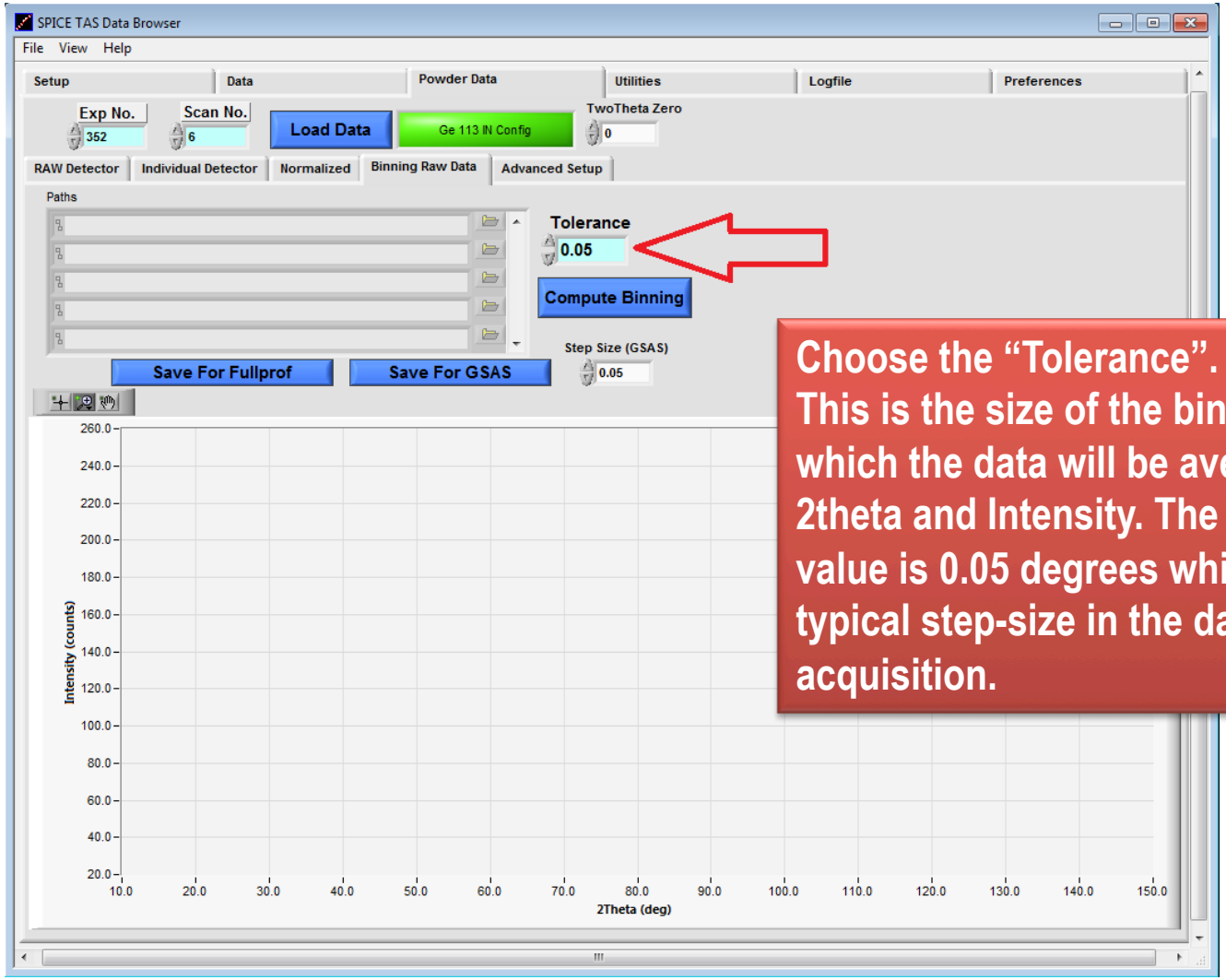
1. Save XYZ File, Press the "OK" Button
2. This is an intermediate file that stitches together the output from all 44 detectors
3. The raw data files "HB2a_exp0#_scan#.dat" and the XYZ files "Scan_#" are saved at the instrument computer at C:\Data\HB2A\exp#\Datafiles\Scan_#.dat

6. Binning the XYZ intermediate file



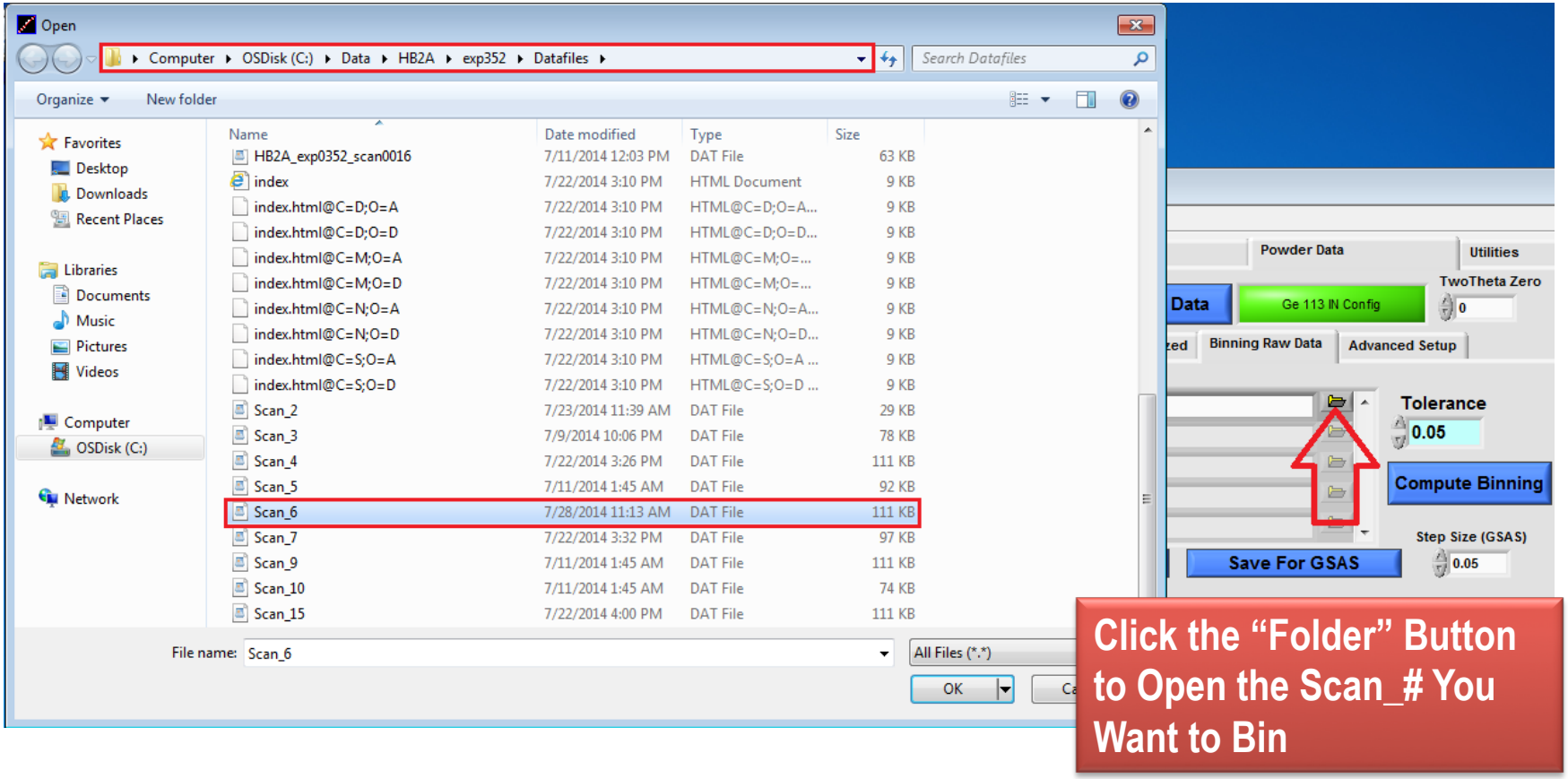
Enter the "Binning Raw Data" Sub-Tab

7. Binning the XYZ intermediate file



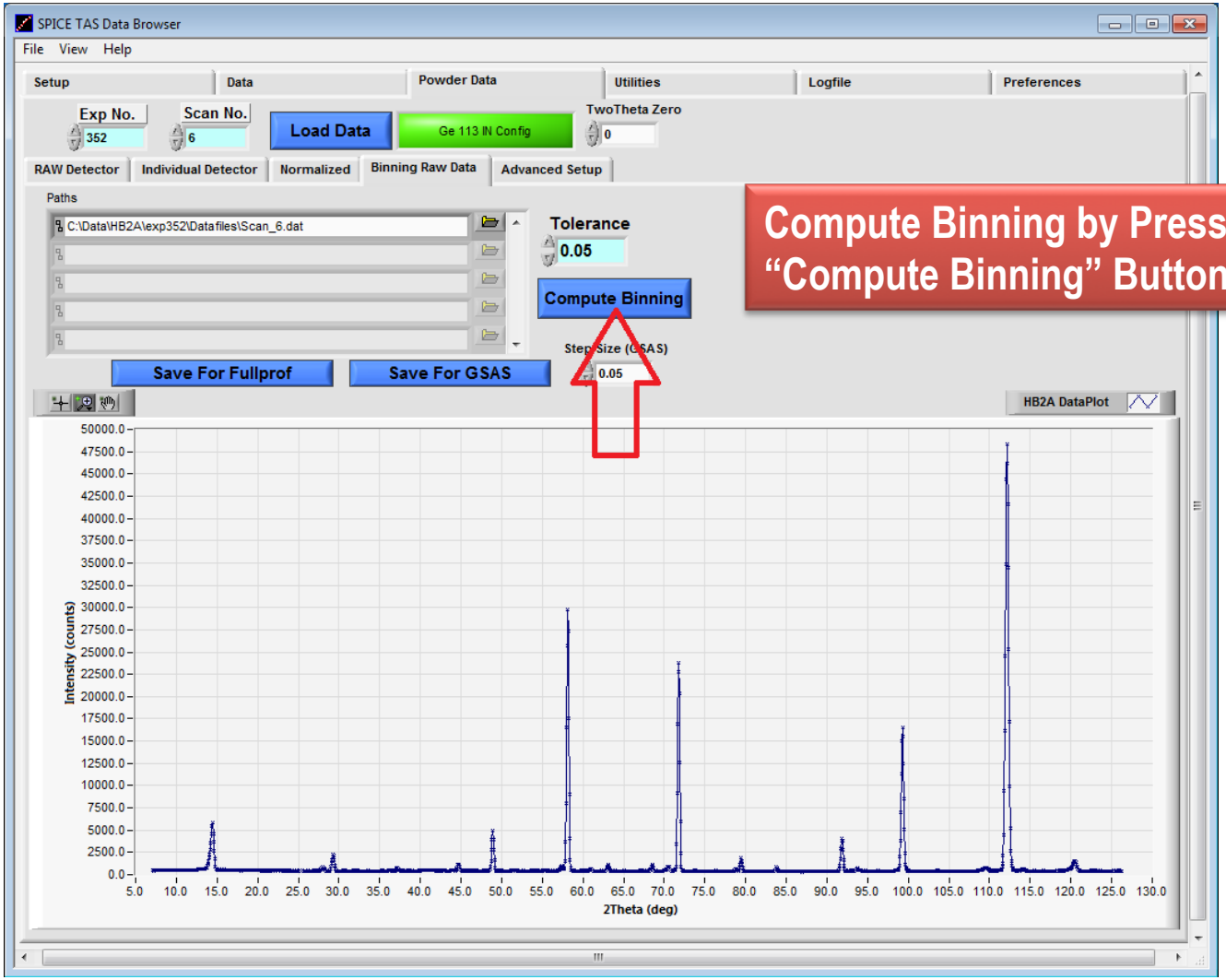
Choose the "Tolerance".
This is the size of the bins within which the data will be averaged in 2theta and Intensity. The default value is 0.05 degrees which is the typical step-size in the data acquisition.

8. Binning Individual scans

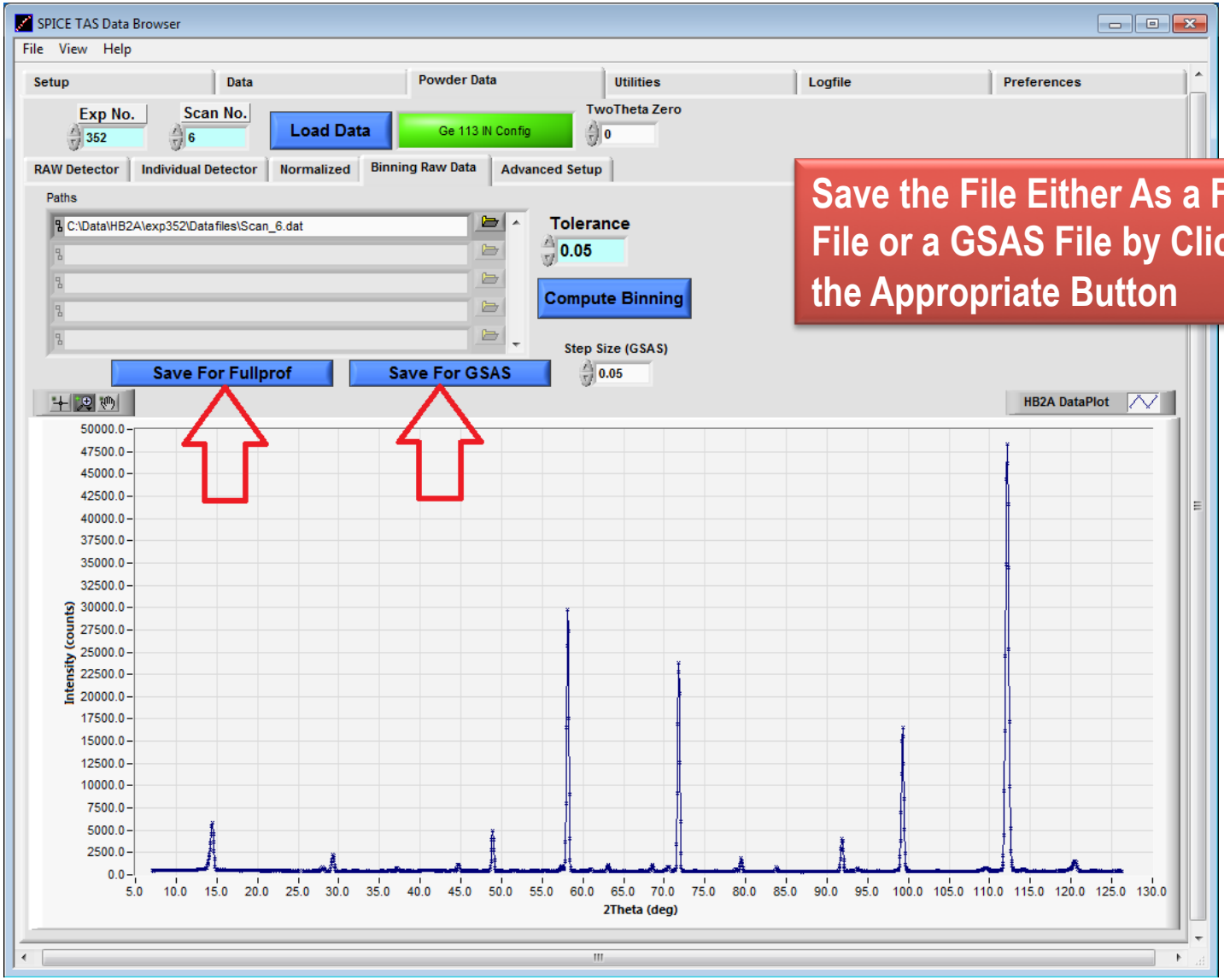


Click the "Folder" Button to Open the Scan_# You Want to Bin

8. Binning Individual scans

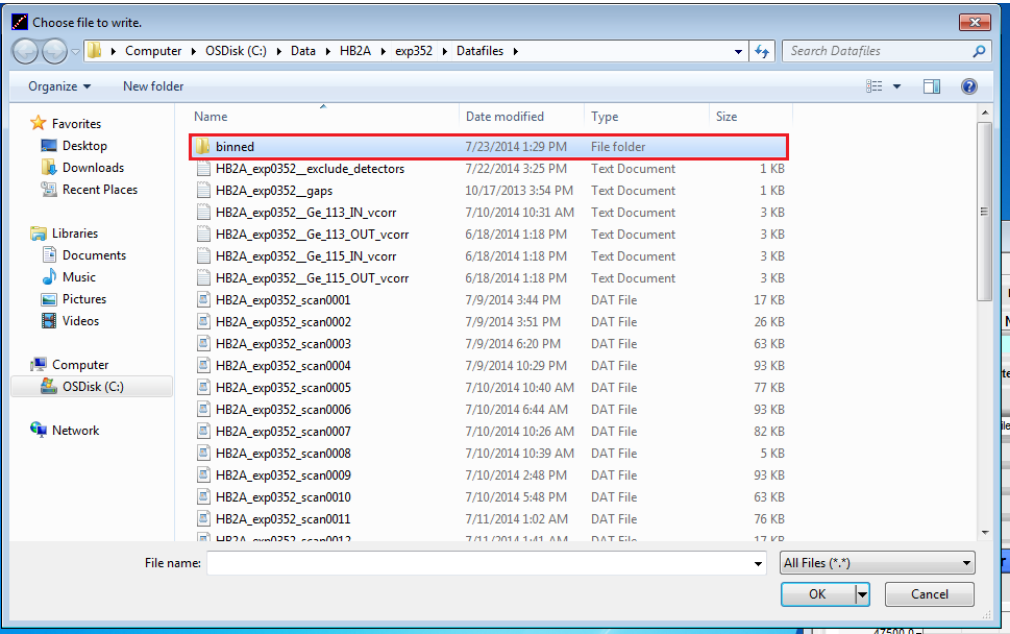


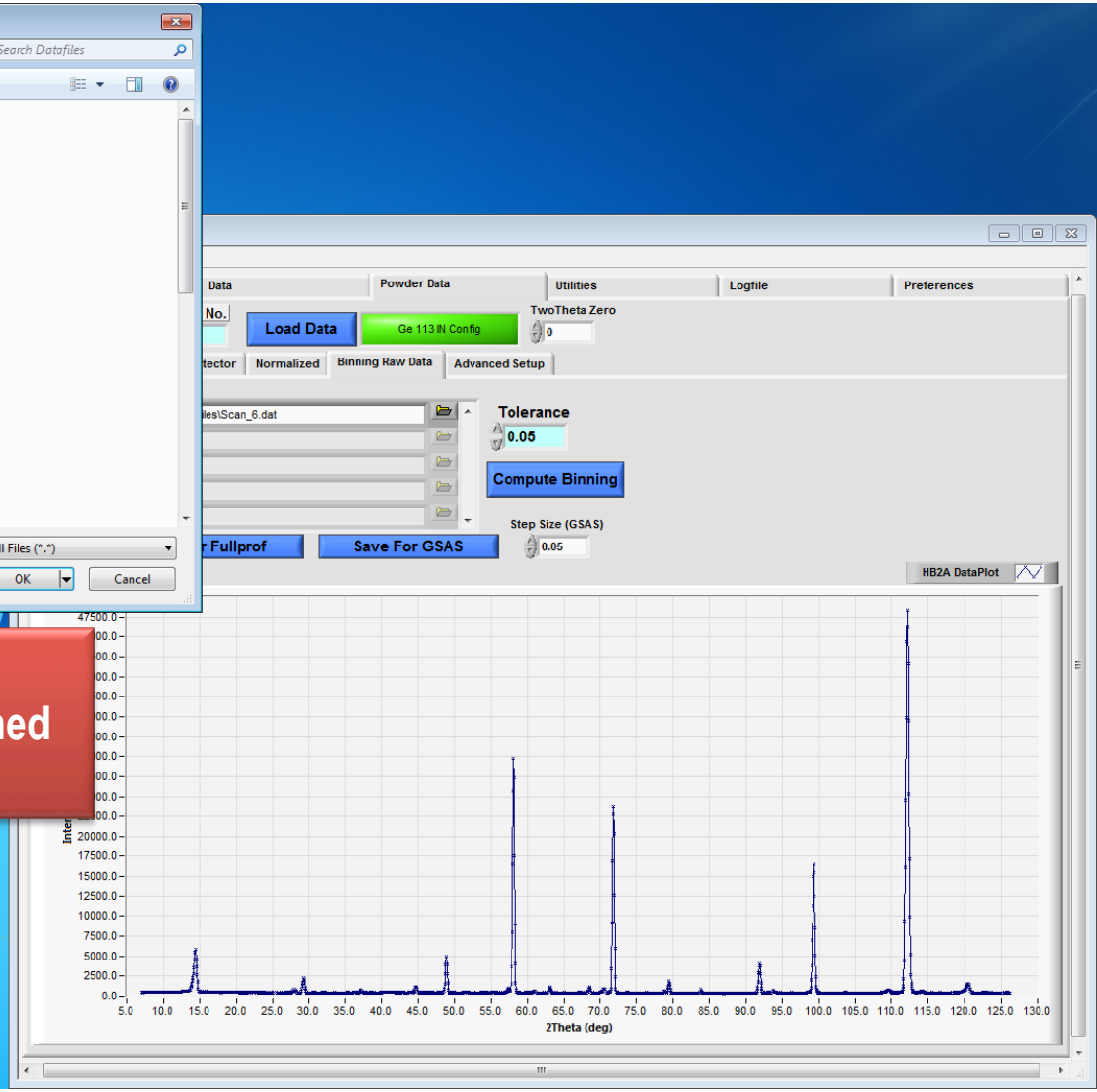
8. Binning individual scans



Save the File Either As a FullProf File or a GSAS File by Clicking the Appropriate Button

9. Saving Binned /Reduced Files

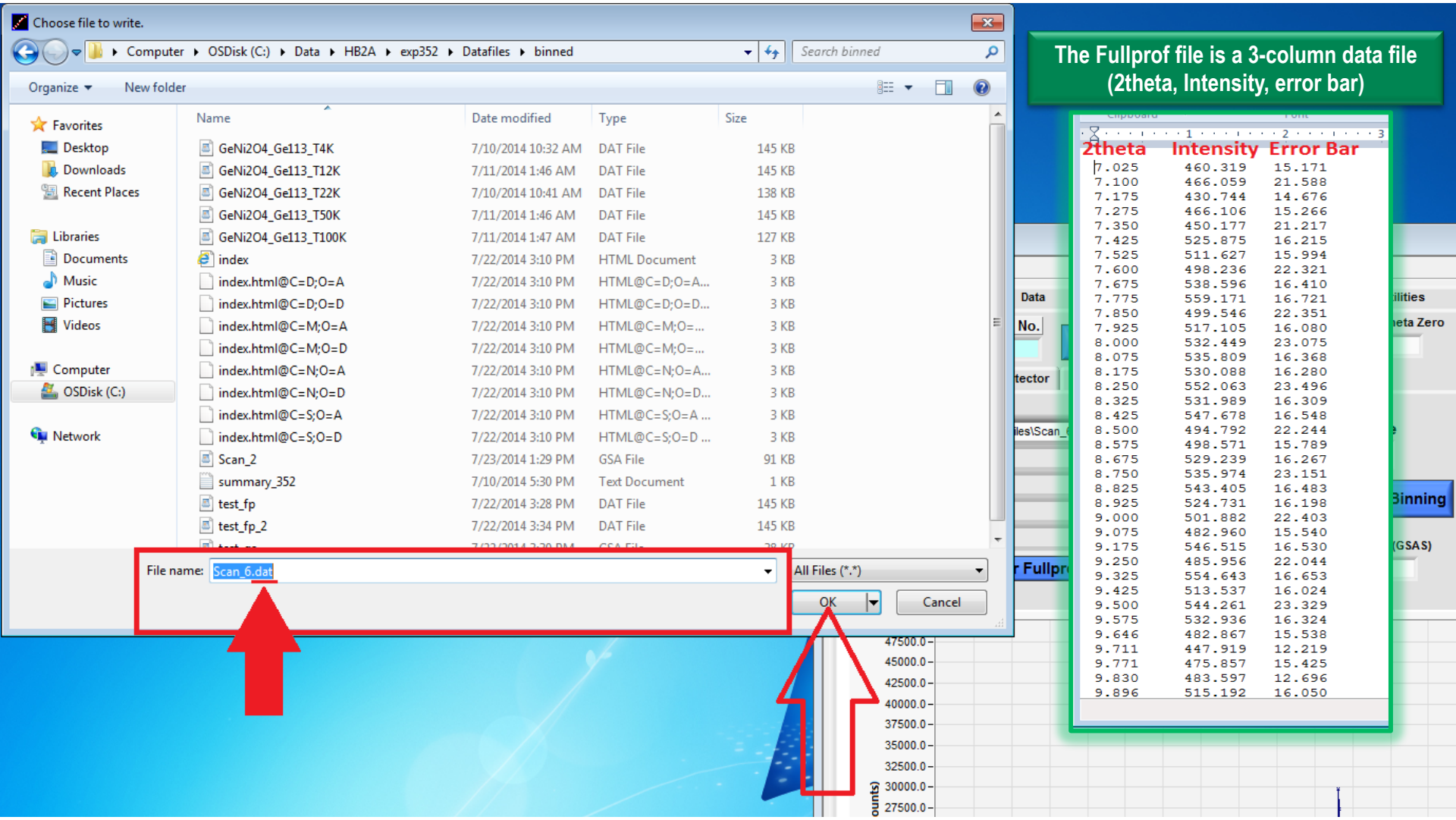




Create a “Binned” folder under “Datafiles” to Save the reduced Binned files in

9. Saving Binned /Reduced Files

To Save as a FullProf File, use the filename extension ".dat"

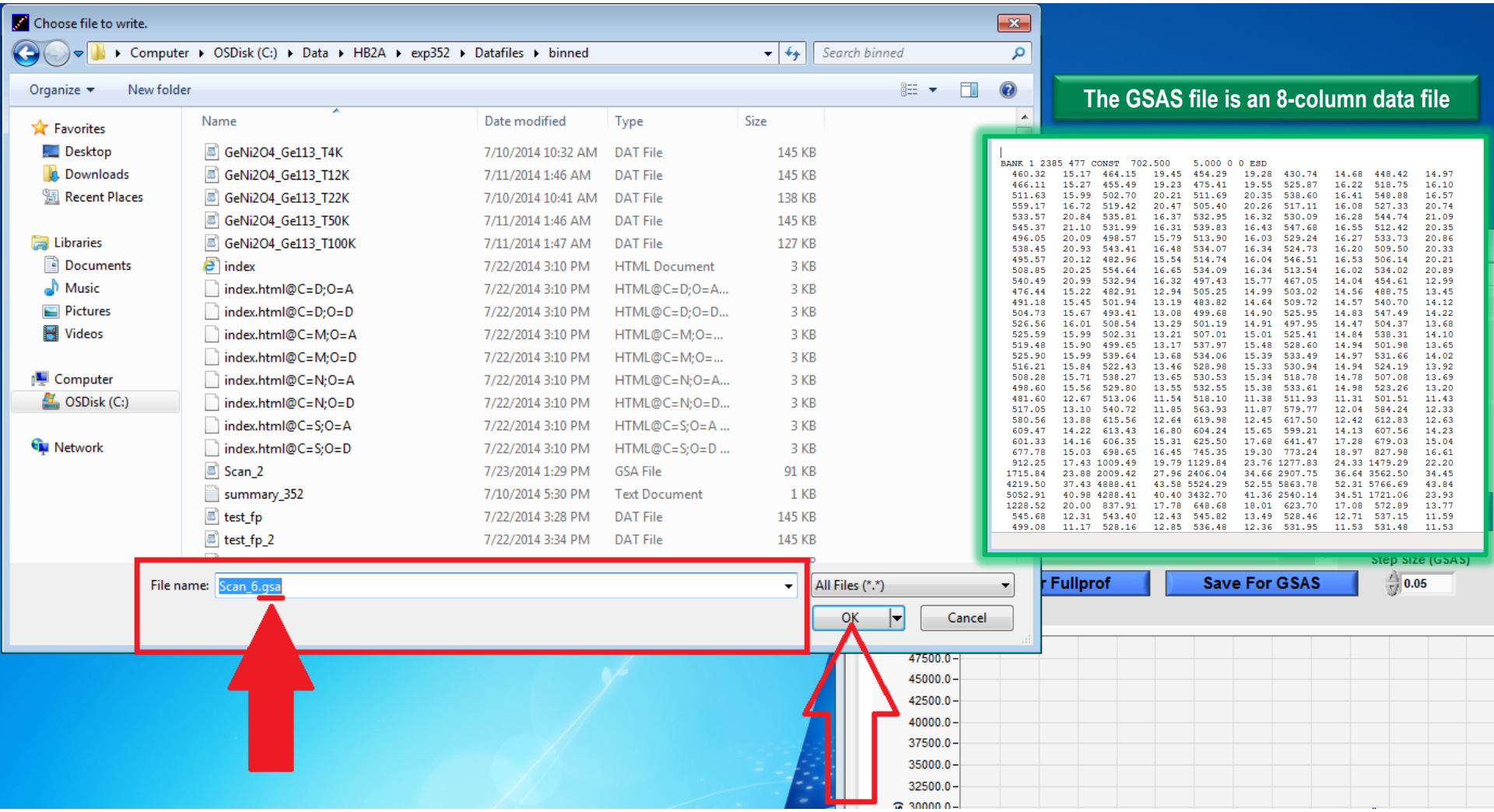


The Fullprof file is a 3-column data file (2theta, Intensity, error bar)

2theta	Intensity	Error Bar
7.025	460.319	15.171
7.100	466.059	21.588
7.175	430.744	14.676
7.275	466.106	15.266
7.350	450.177	21.217
7.425	525.875	16.215
7.525	511.627	15.994
7.600	498.236	22.321
7.675	538.596	16.410
7.775	559.171	16.721
7.850	499.546	22.351
7.925	517.105	16.080
8.000	532.449	23.075
8.075	535.809	16.368
8.175	530.088	16.280
8.250	552.063	23.496
8.325	531.989	16.309
8.425	547.678	16.548
8.500	494.792	22.244
8.575	498.571	15.789
8.675	529.239	16.267
8.750	535.974	23.151
8.825	543.405	16.483
8.925	524.731	16.198
9.000	501.882	22.403
9.075	482.960	15.540
9.175	546.515	16.530
9.250	485.956	22.044
9.325	554.643	16.653
9.425	513.537	16.024
9.500	544.261	23.329
9.575	532.936	16.324
9.646	482.867	15.538
9.711	447.919	12.219
9.771	475.857	15.425
9.830	483.597	12.696
9.896	515.192	16.050

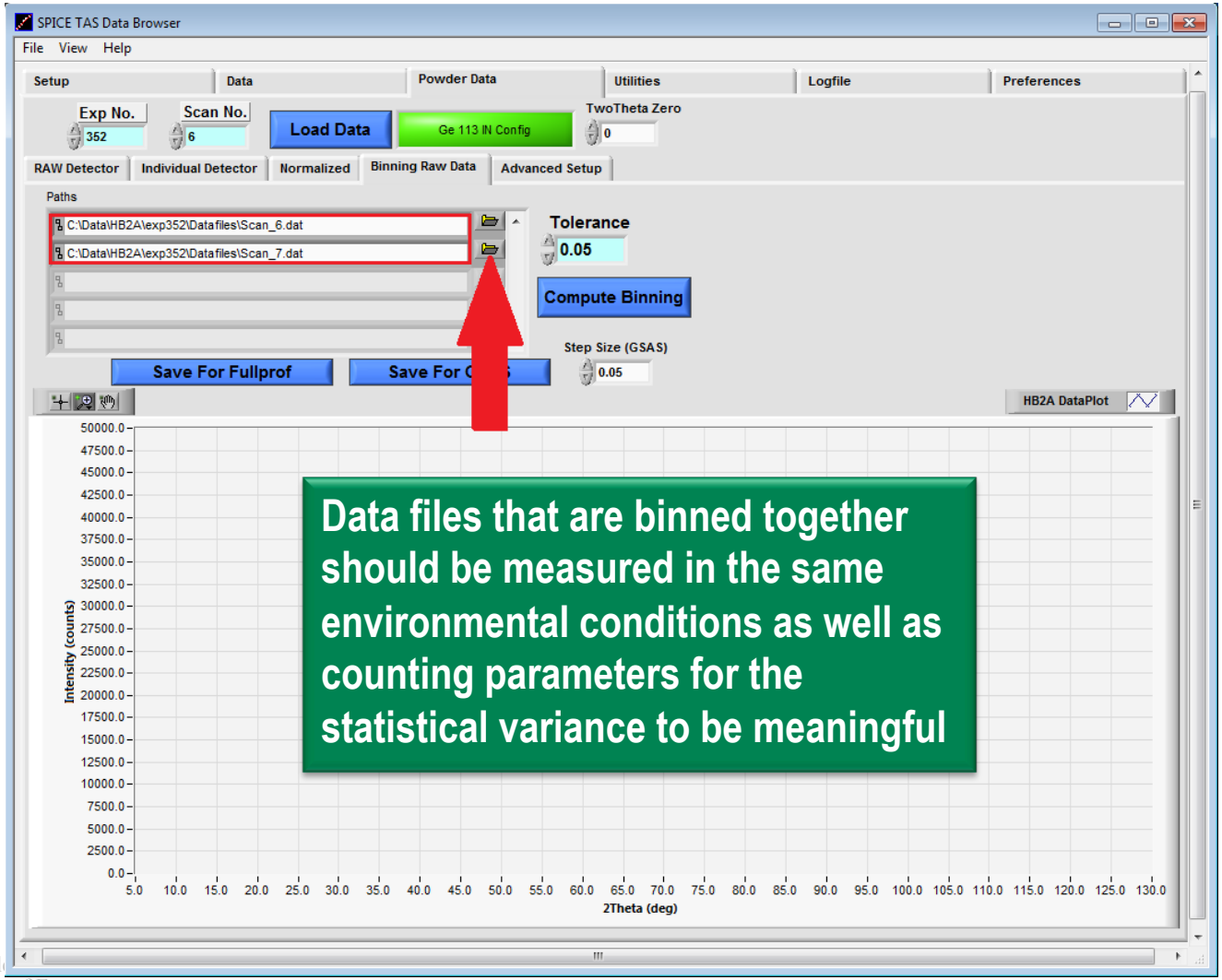
9. Saving Binned /Reduced Files

To Save as GSAS File, use the filename extension ".gsa"



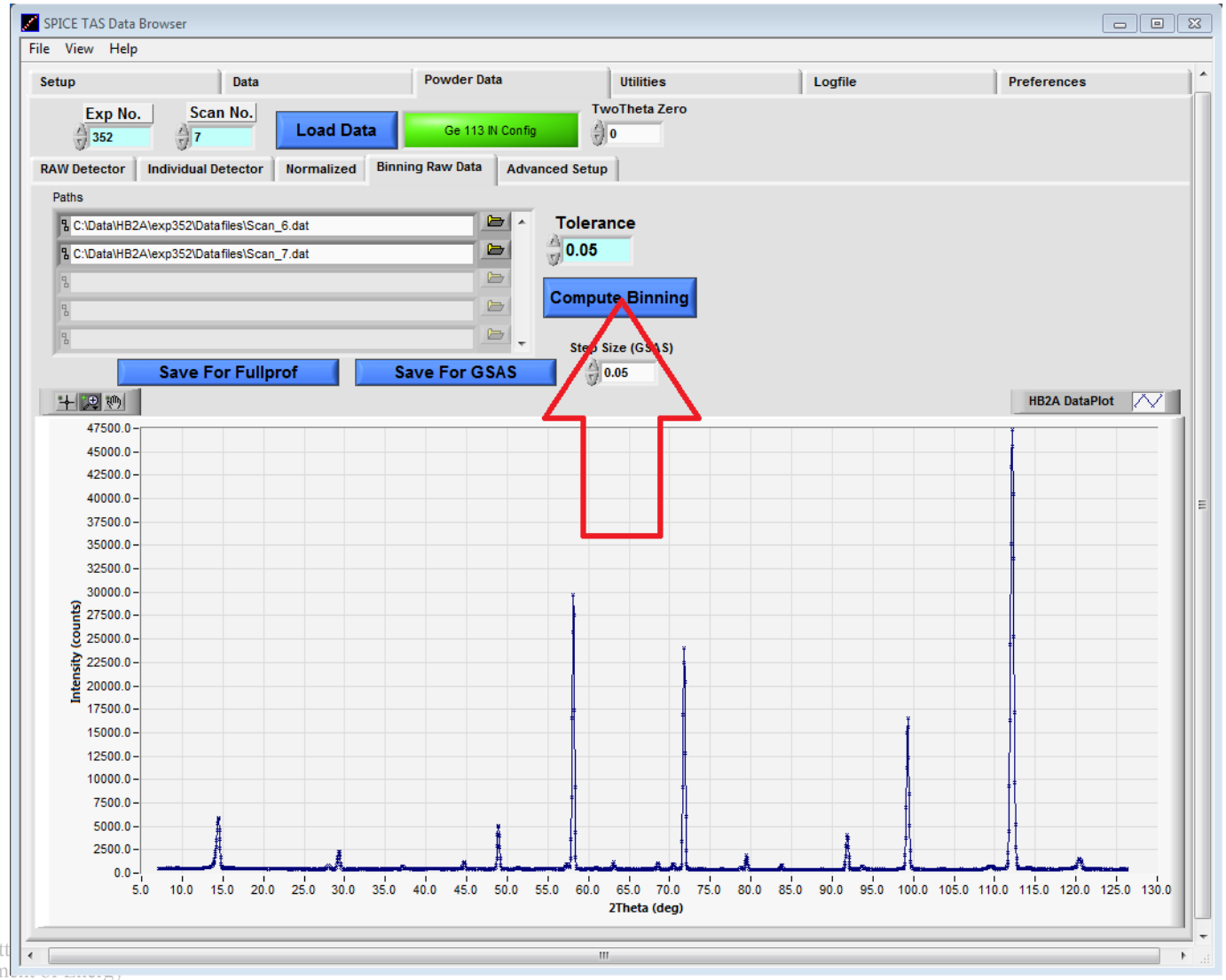
10. Binning Multiple scans

Click each of the "Folder" Button to Open the intermediate XYZ files "Scan_#" you want to Bin

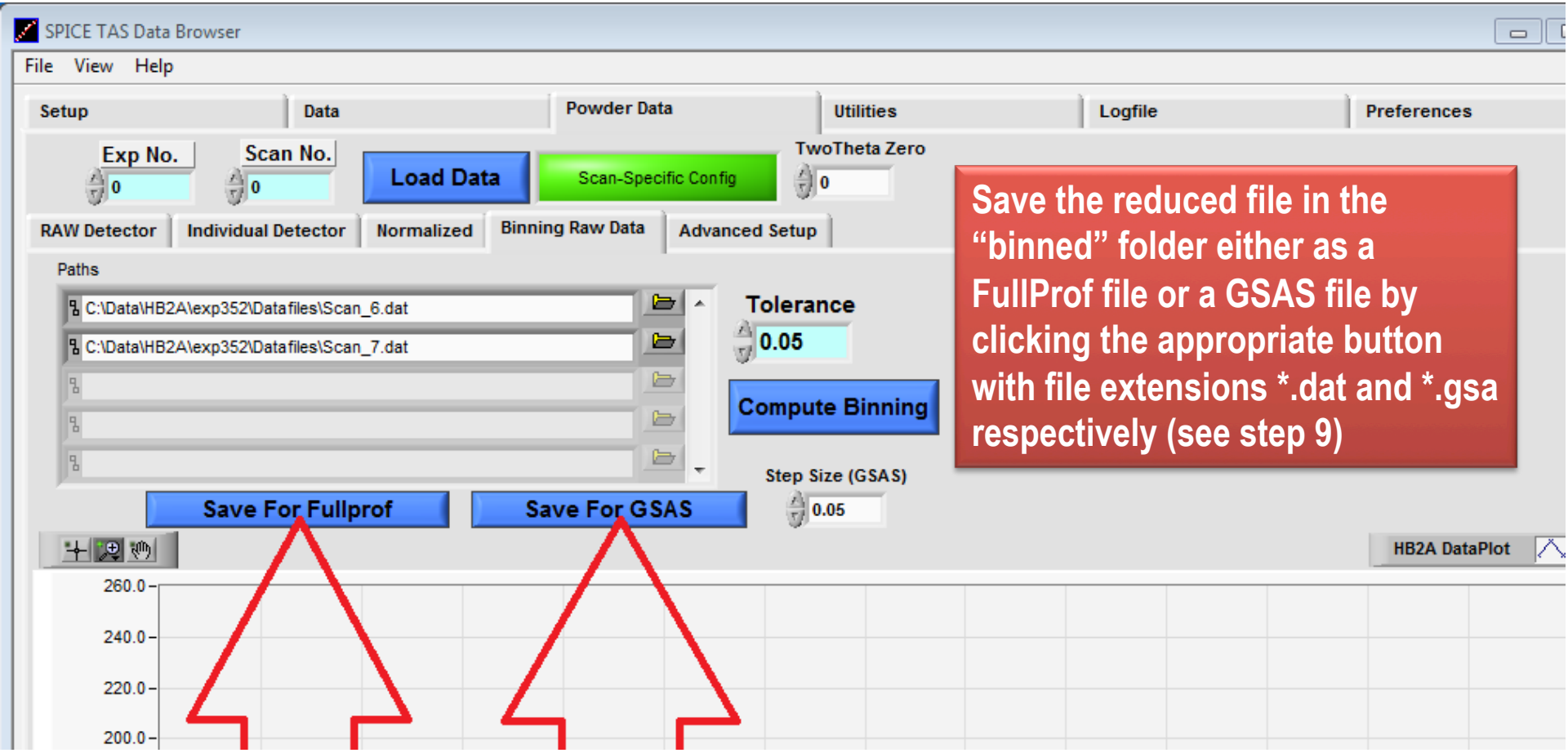


10. Binning multiple scans

Compute Binning by Pressing the "Compute Binning" Button



11. Saving reduced/binned files from multiple scans



Save the reduced file in the "binned" folder either as a FullProf file or a GSAS file by clicking the appropriate button with file extensions *.dat and *.gsa respectively (see step 9)