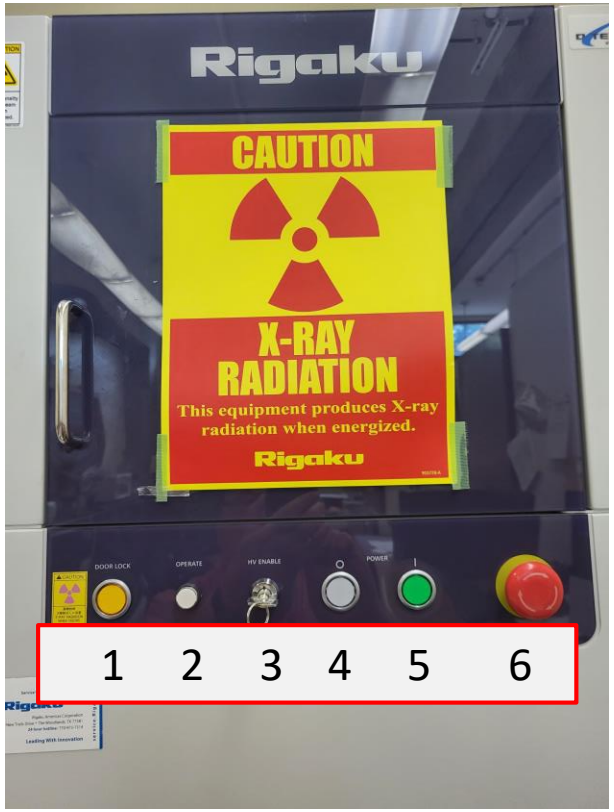
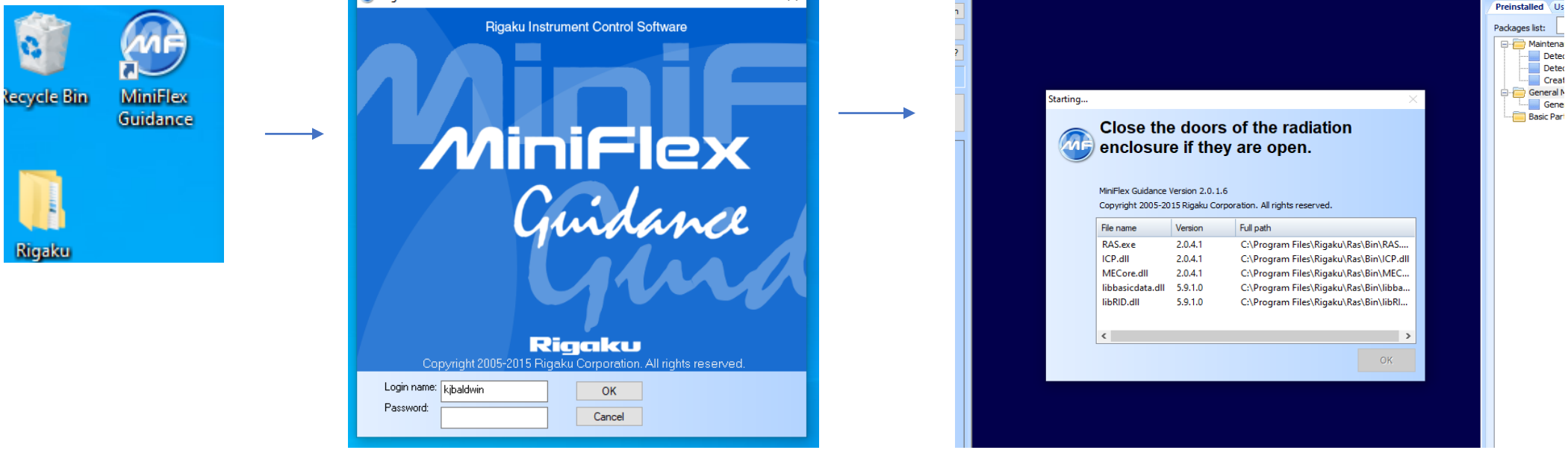
MiniFlex 600

1. Sign the log sheet. When finished be sure to enter the total time in decimal hours.
2. Log onto the control computer using your NetID /password.
3. Turn on the diffractometer. Press the **On** button then the Door access button to stop the beeping sound.

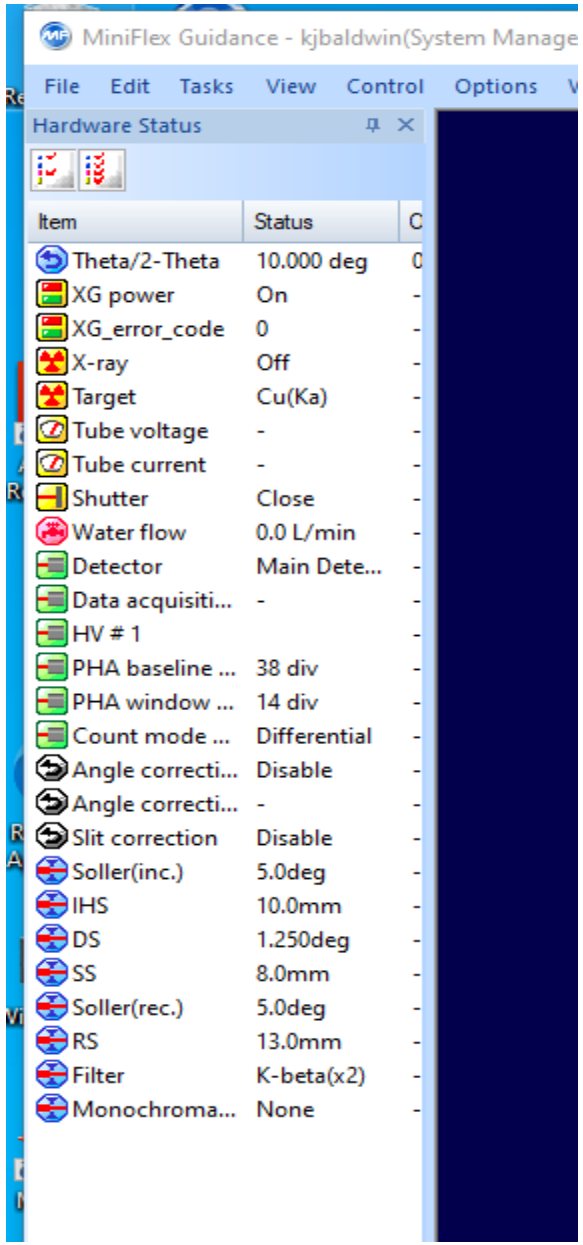


1 – Door access. When flashing and beeping door is unlocked.
2 – Indicator light
3 – Enable/Disable key. When key is removed diffractometer is disabled
4 – Off button
5 – On button
6 – Emergency Stop Button

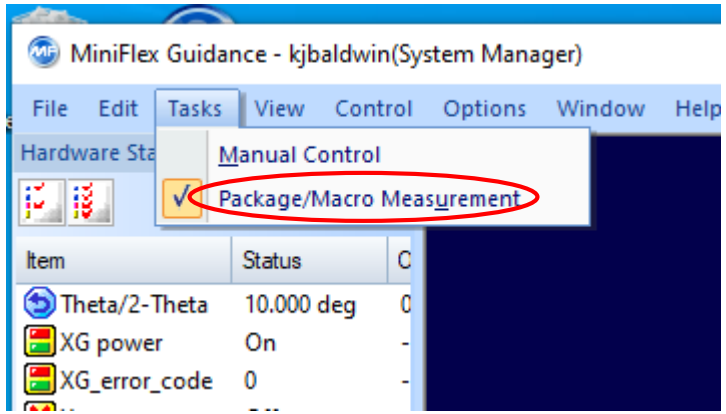
4. Start the control program. Double click MiniFlex Guidance on the desktop. The MinFlex Guidance login screen will appear with your NetID as the default Login name. Click OK. The MiniFlex *Starting* window will appear as the system initializes.

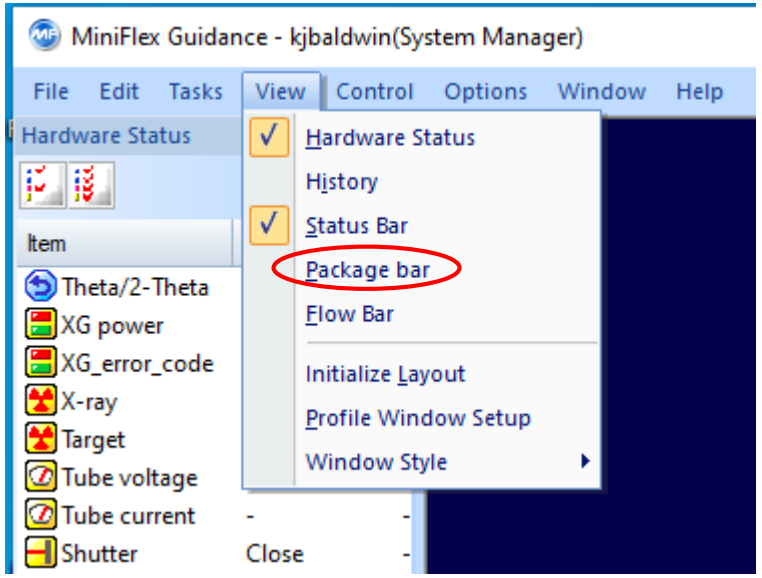


5. Once the system has initialized the main window will open.

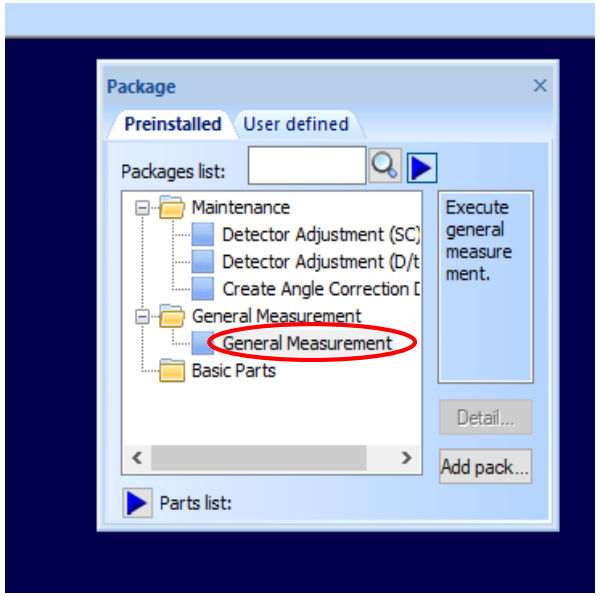


6. Select *Tasks → Package/Macro Management* and *View → Package Bar*



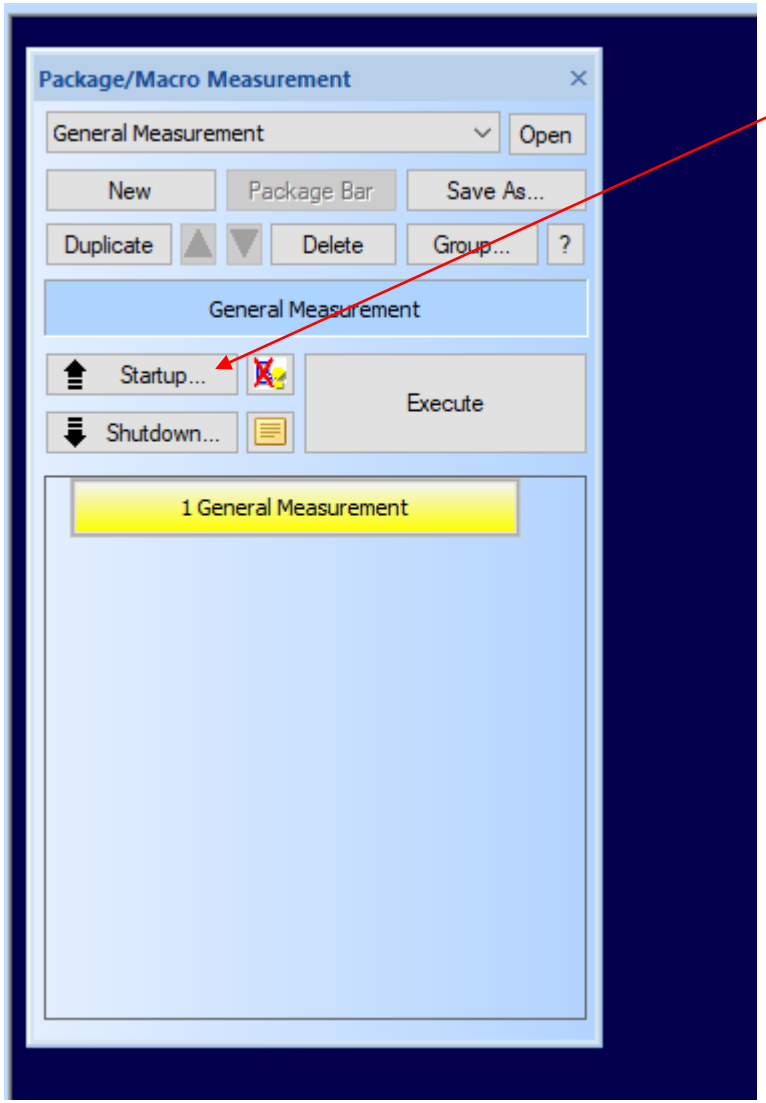


7. When the *Package* window opens double click *General Measurement*

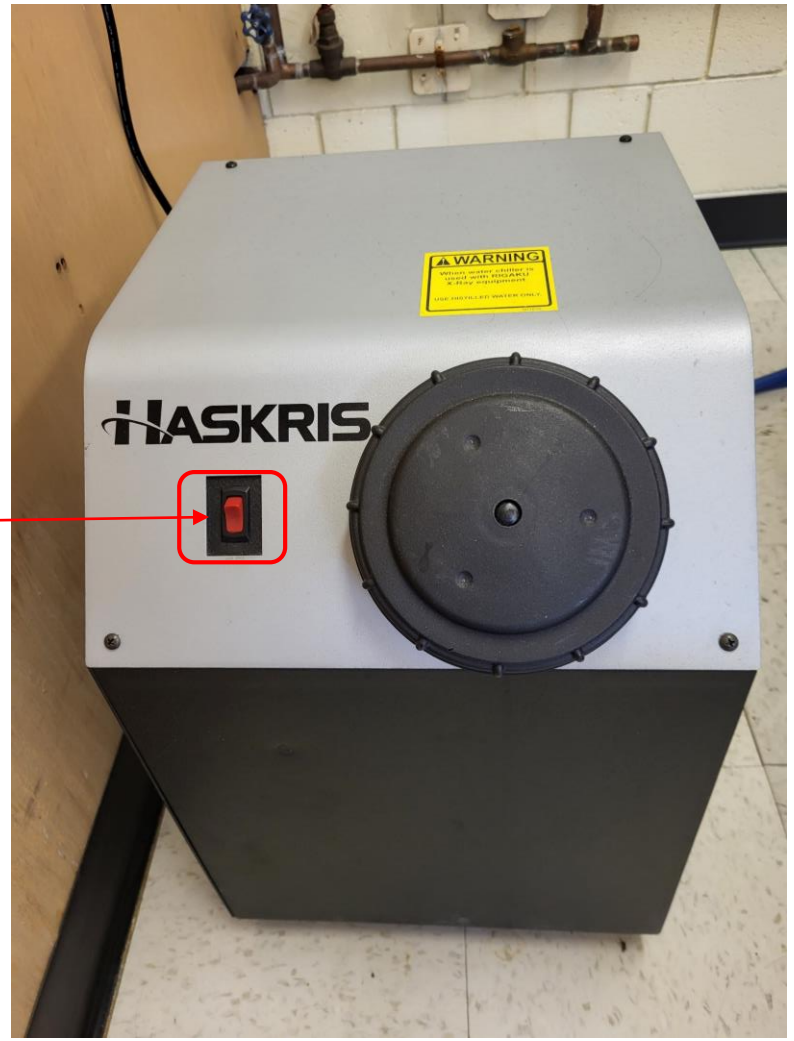


If you exit the program correctly, steps 6 and 7 will be remembered and will not have to be repeated the next time you run *MiniFlex Guidance*.

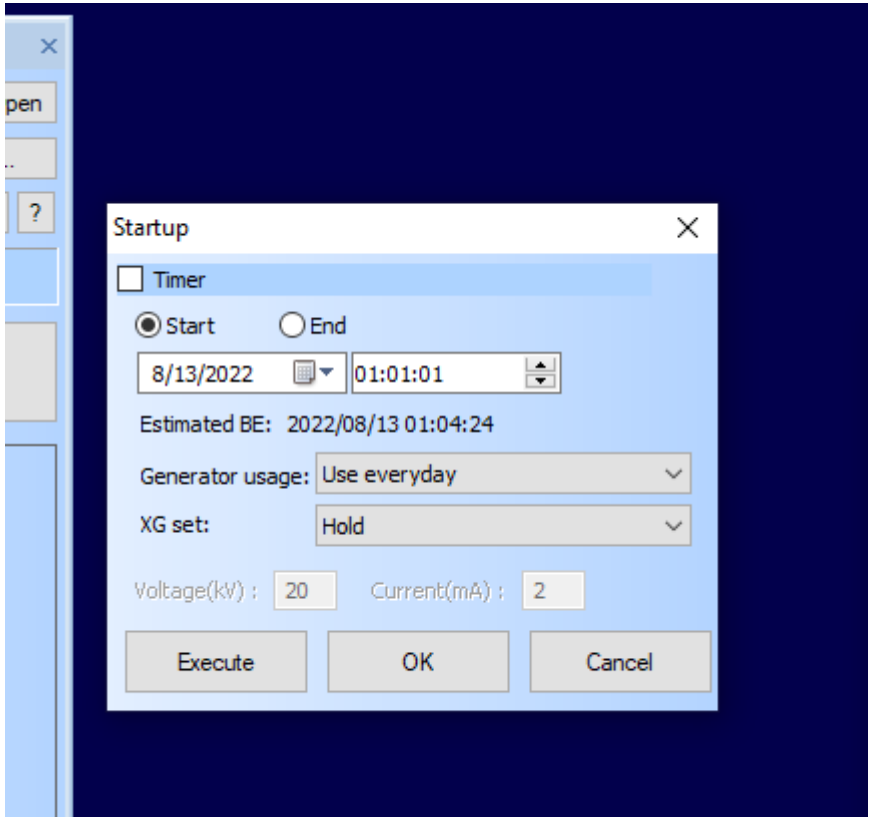
8. The *Package/Macro Measurement* window will open.

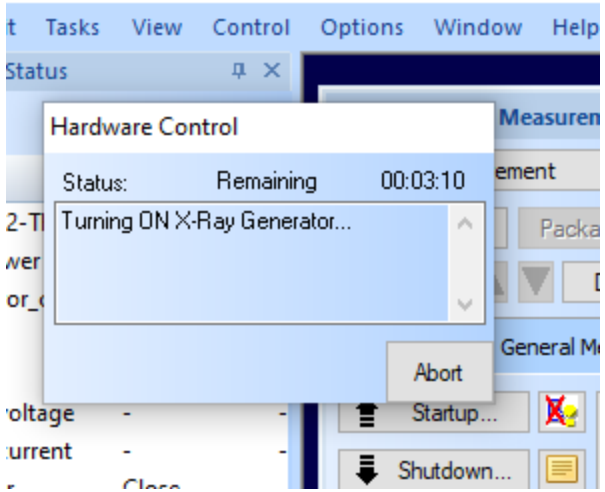


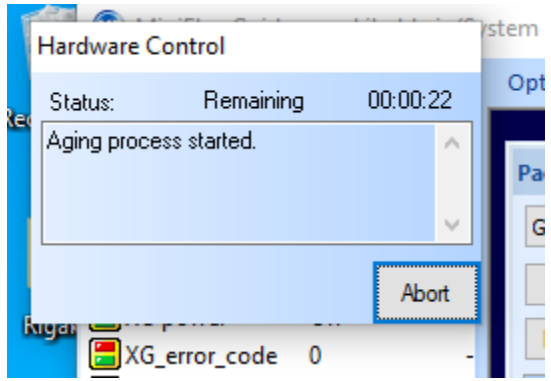
9. Turning on the x-ray generator. Turn on the Haskris heat exchanger then click Startup in the *Package/Macro Measurement* window.



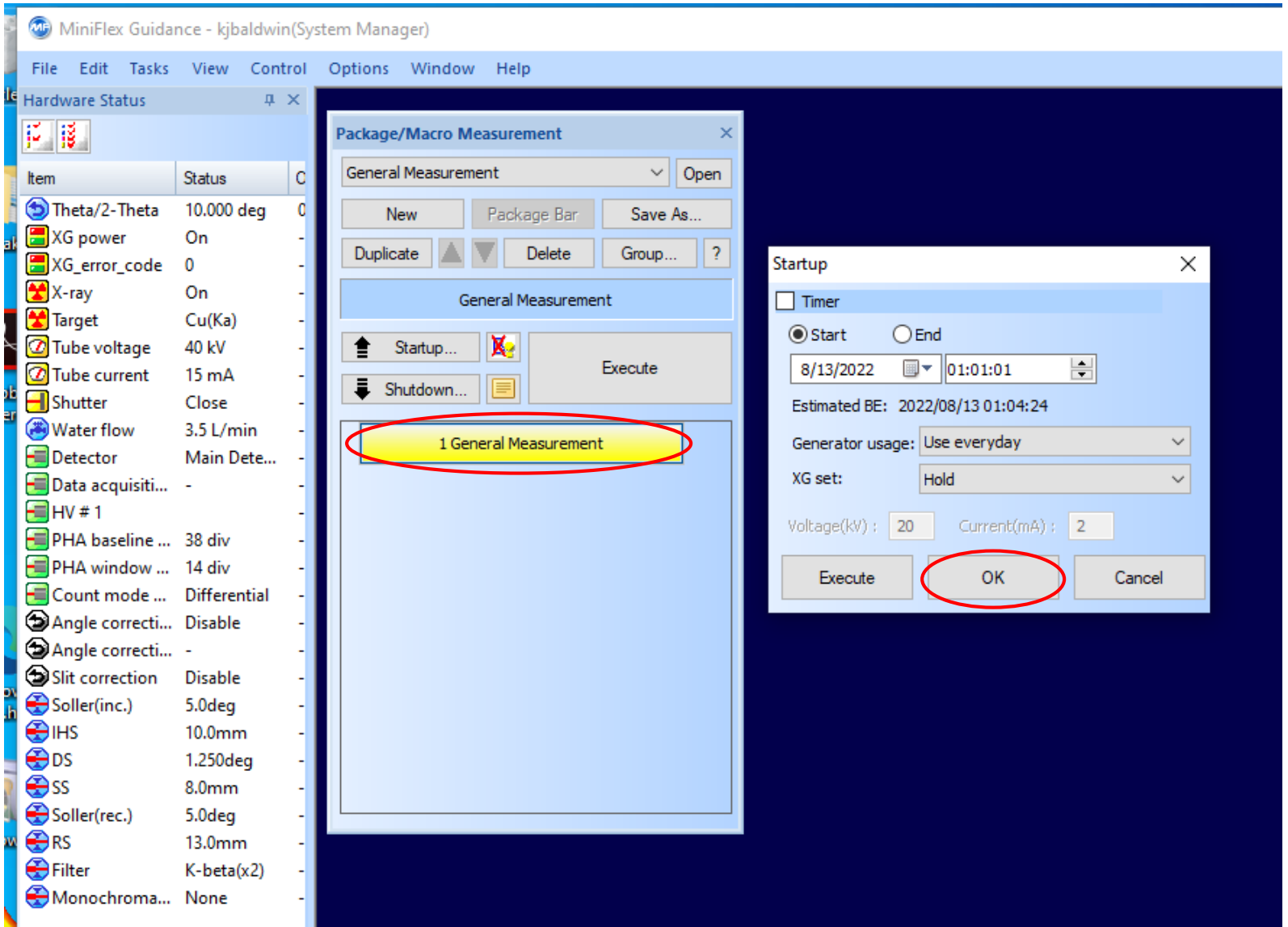
10. The generator *Startup* window will open. Leave *Generator usage:* as *Use everyday* and click *Execute.* The *Turning On X-ray Generator* message will popup followed by *Aging process started.* This will take a few minutes.



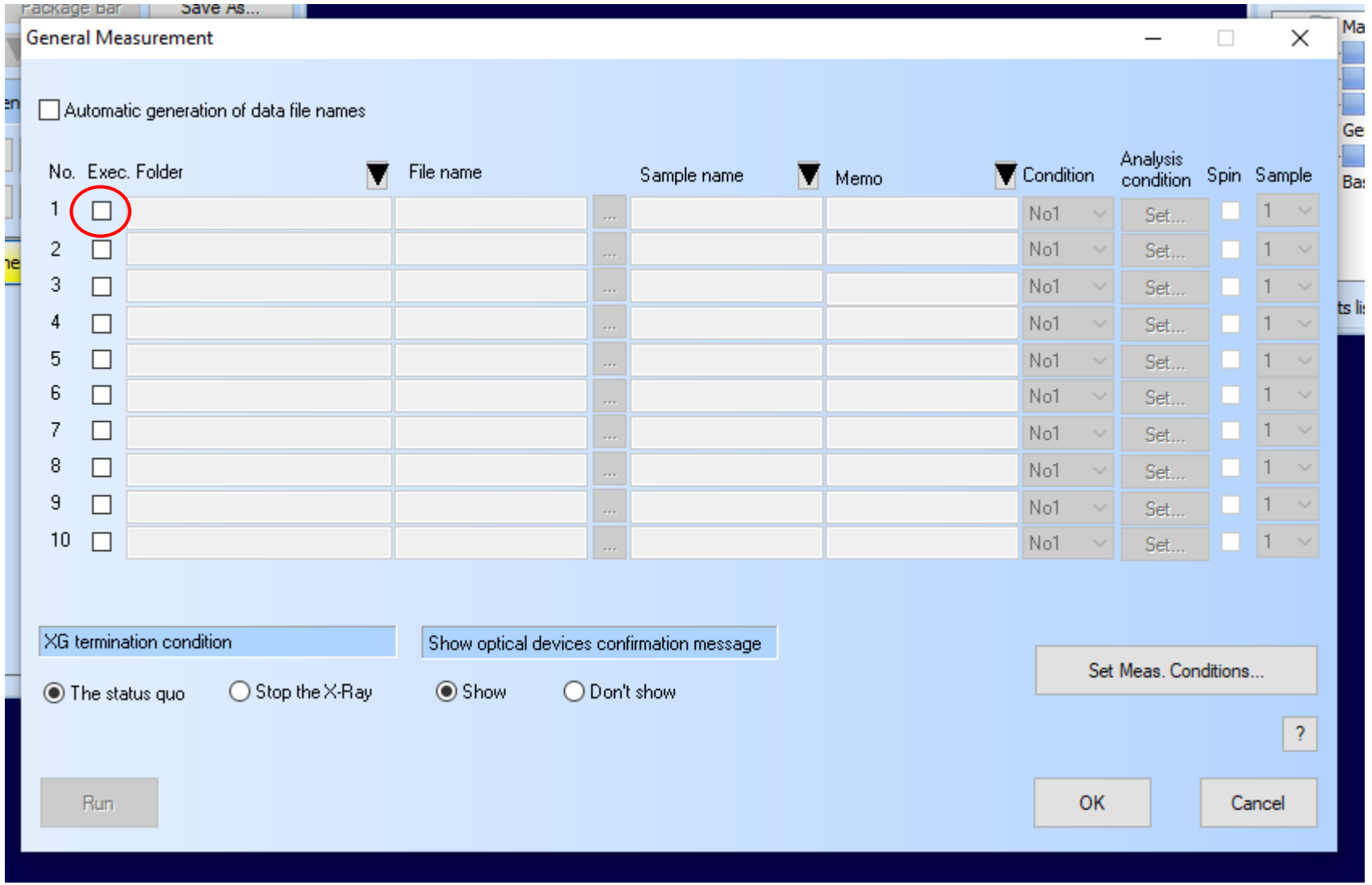




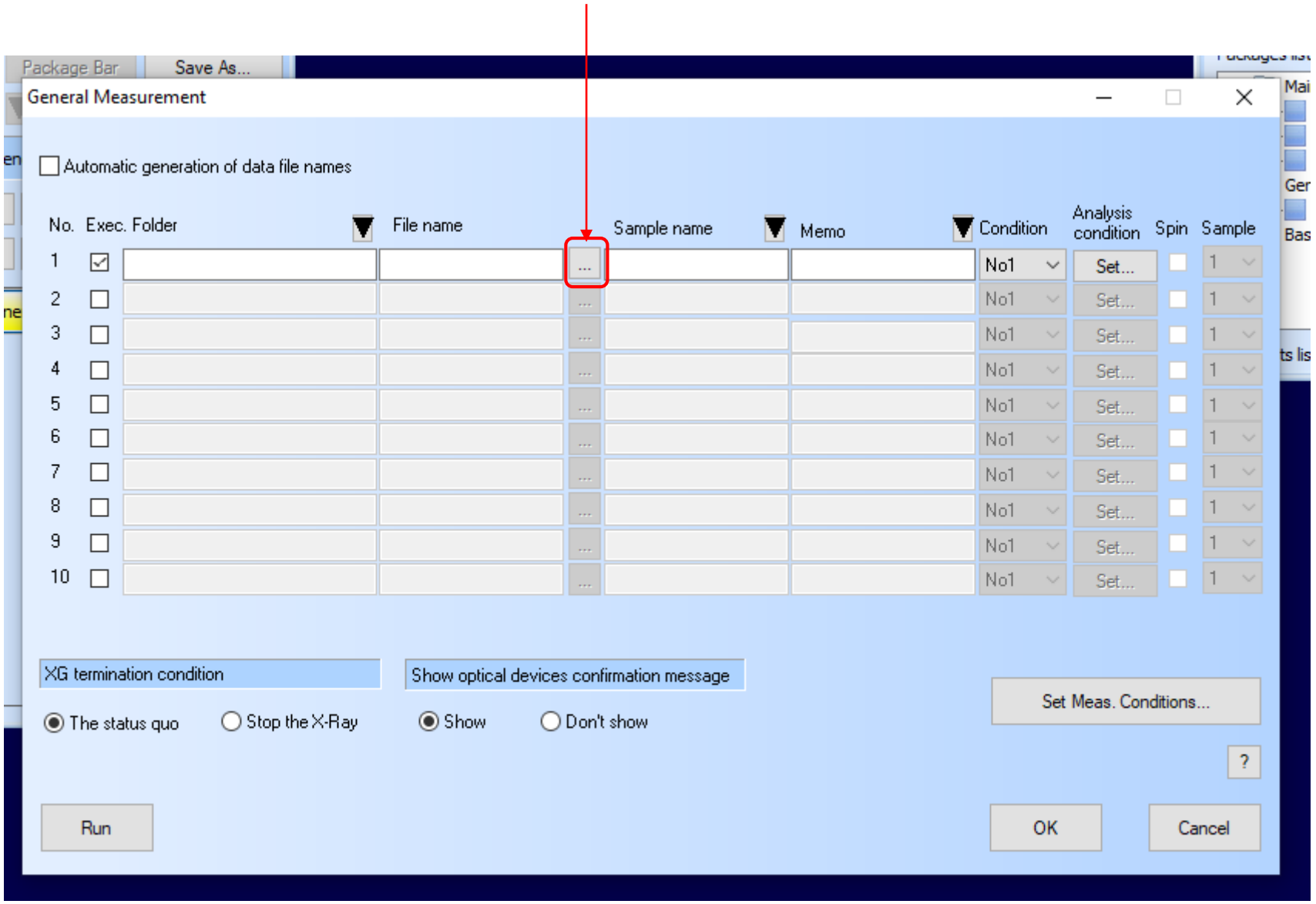
11.When the generator is on and ready you can click *OK* in the *Startup* window then *1 General Measurement* in *Package/Macro Measurement* window



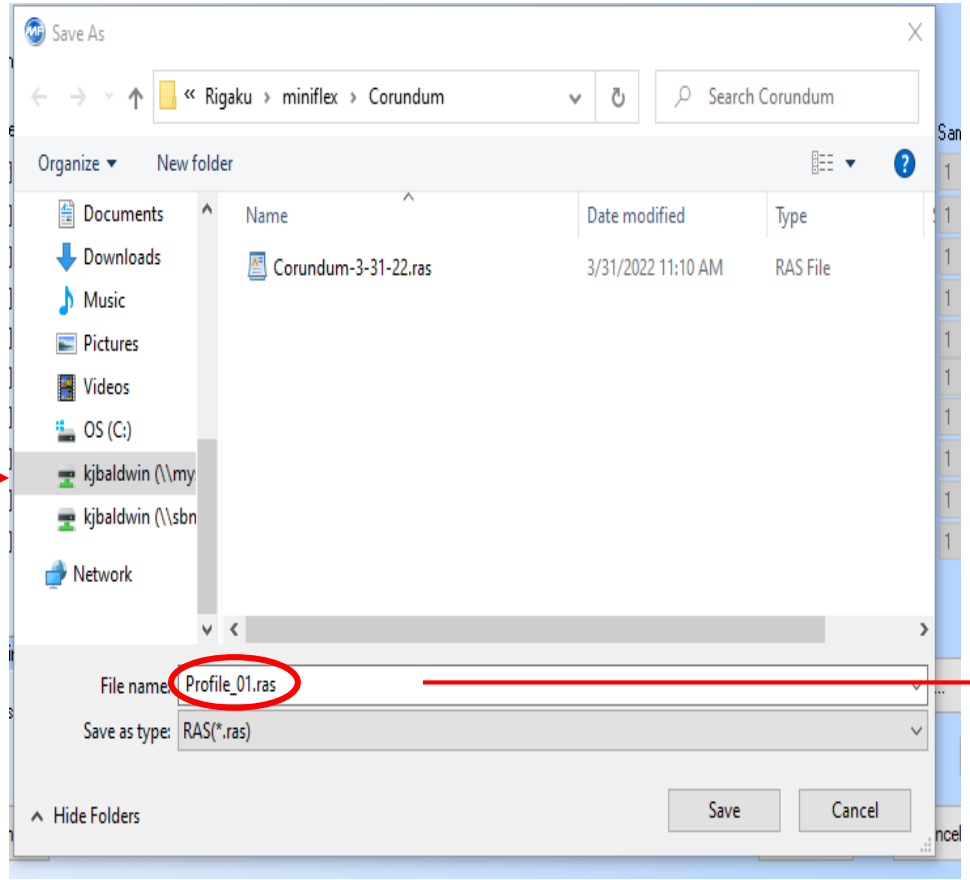
12a *General Measurement*　Check the first check box.

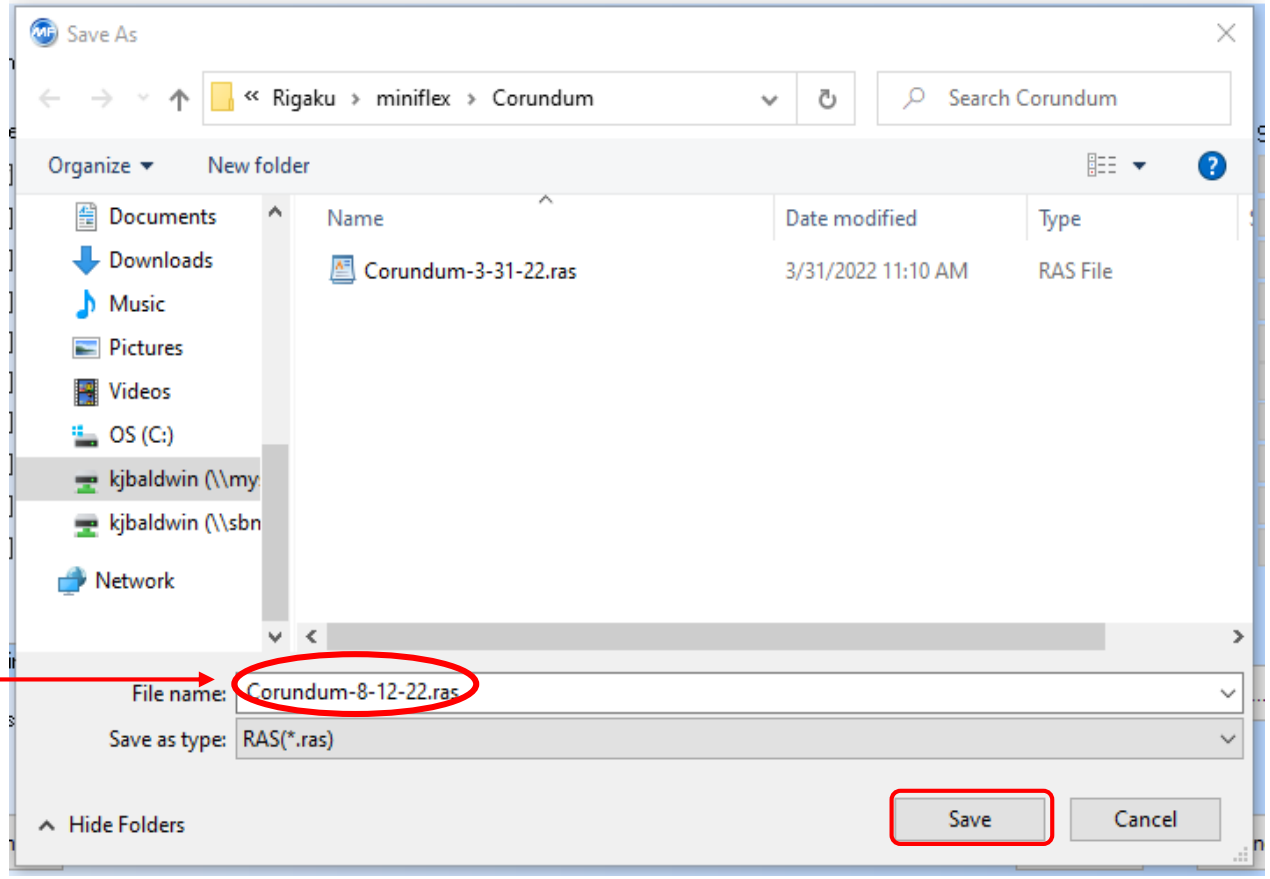


12b *General Measurement* continued. Click the navigation button..

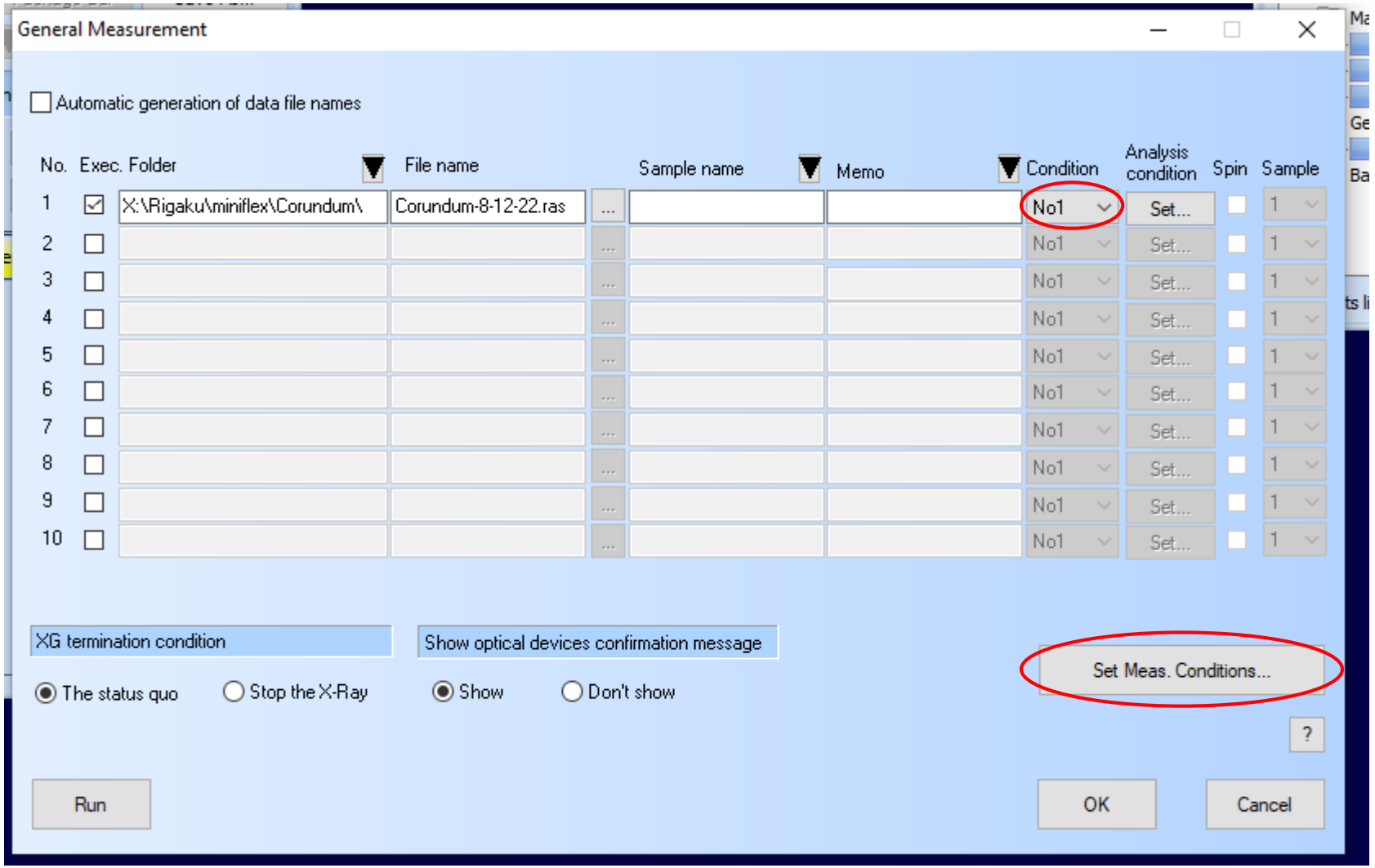


12c Navigate to mysbfiles and enter an appropriate filename and click *Save*

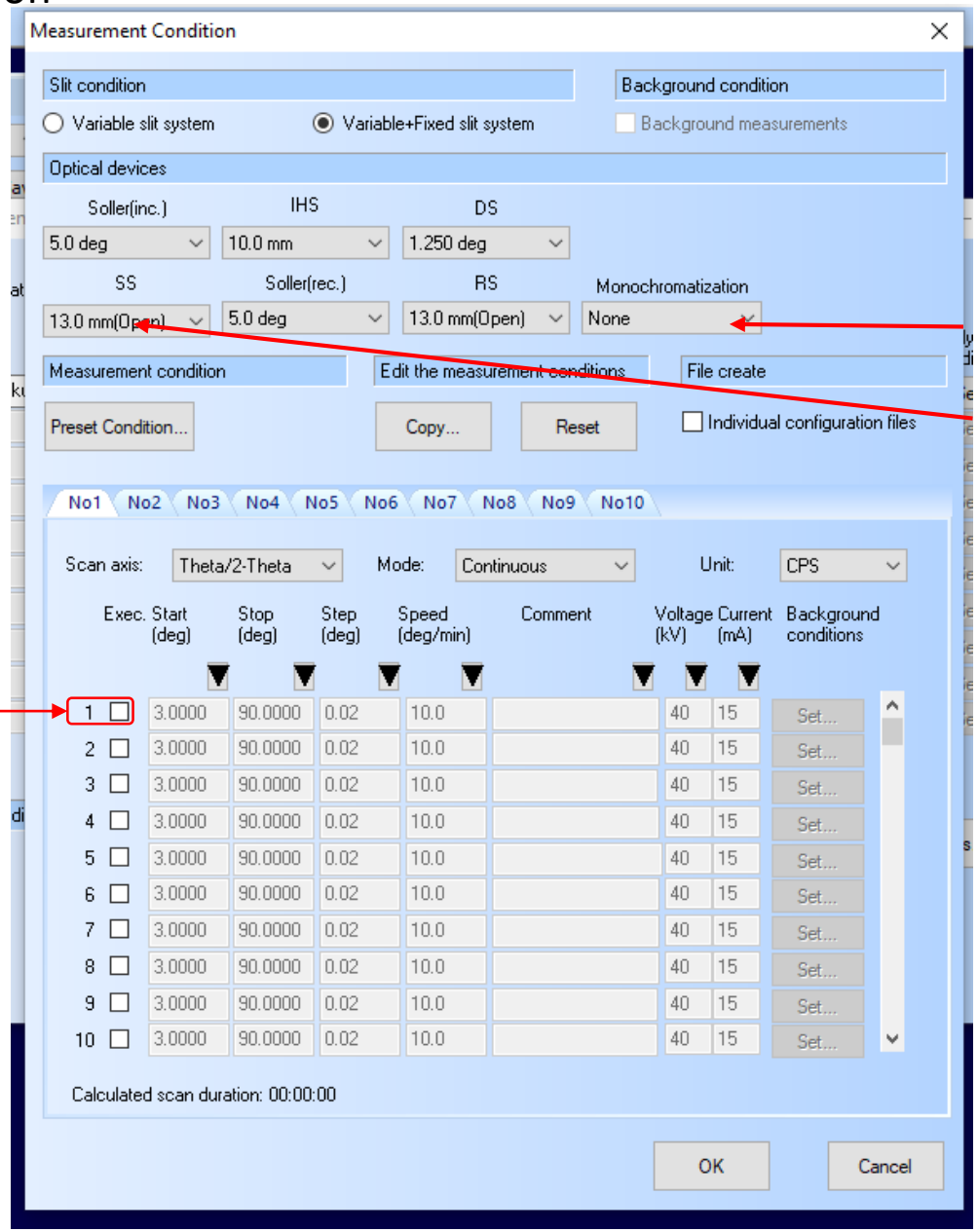




12d *General Measurement* continued. *Sample name* and *Memo* are text fields, enter any information you want or they may be left blank. Leave *Condition* as *No1* and click *Set Meas. Conditions…*



13a Measurement Condition



Make the following changes so this information matches the physical setup of the diffractometer.

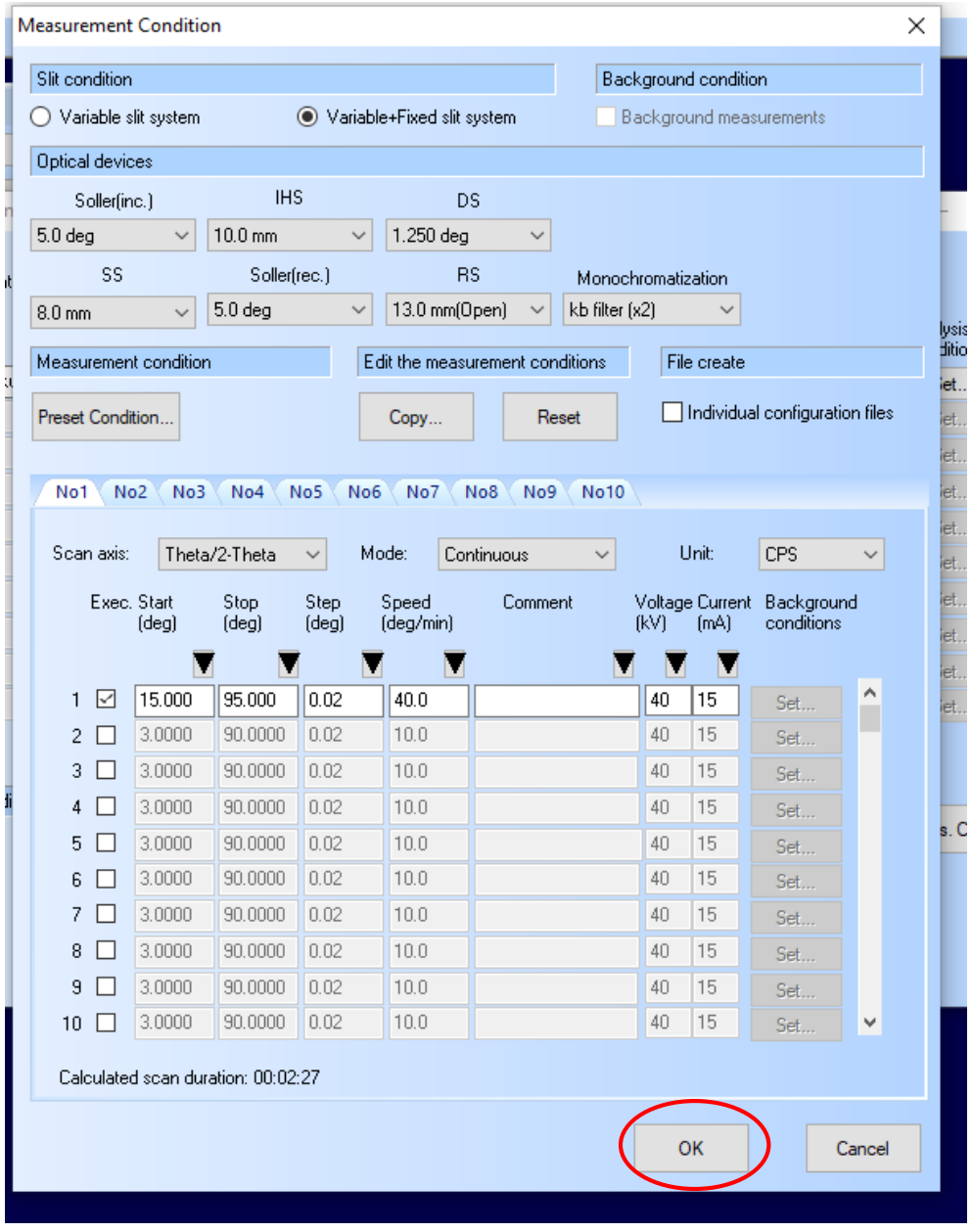
Change *Monochromatization* to *kb filter (x2)*

Change SS to 8.0 mm

If you exit the program correctly, these changes will be remembered and will not have to be repeated the next time you run *MiniFlex Guidance*.

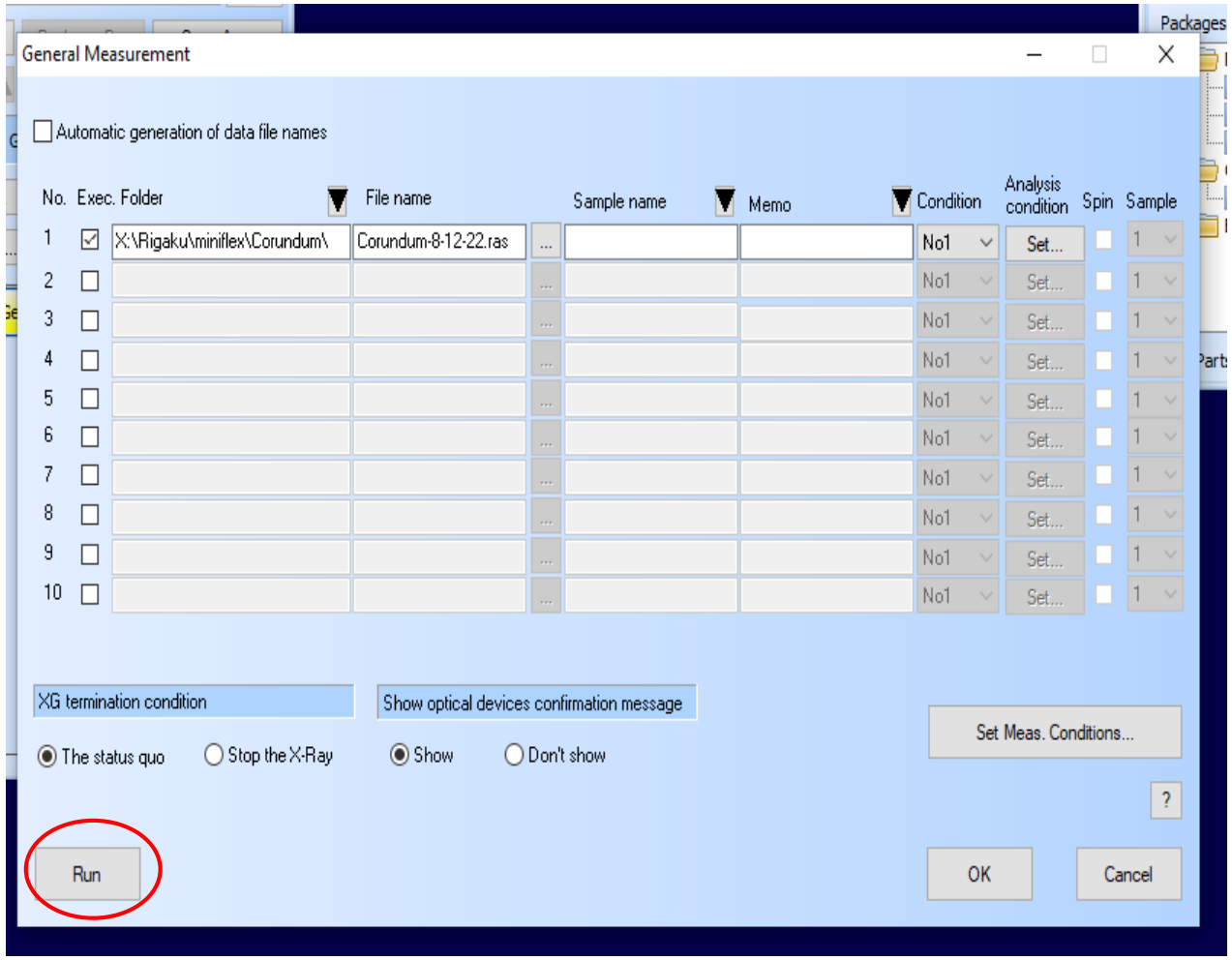
Check *box 1* and enter appropriate values for *Start Stop* and *Speed.* Leave *Step* as 0.02

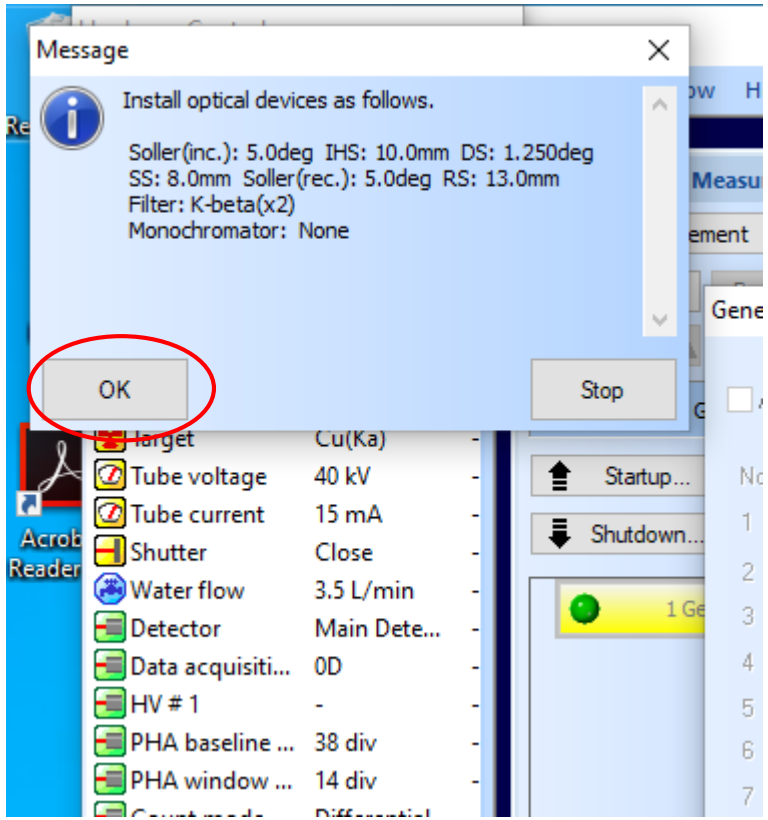
13b Measurement Condition continued. Click *OK* and *General Measurement* panel will open. But first load the sample.



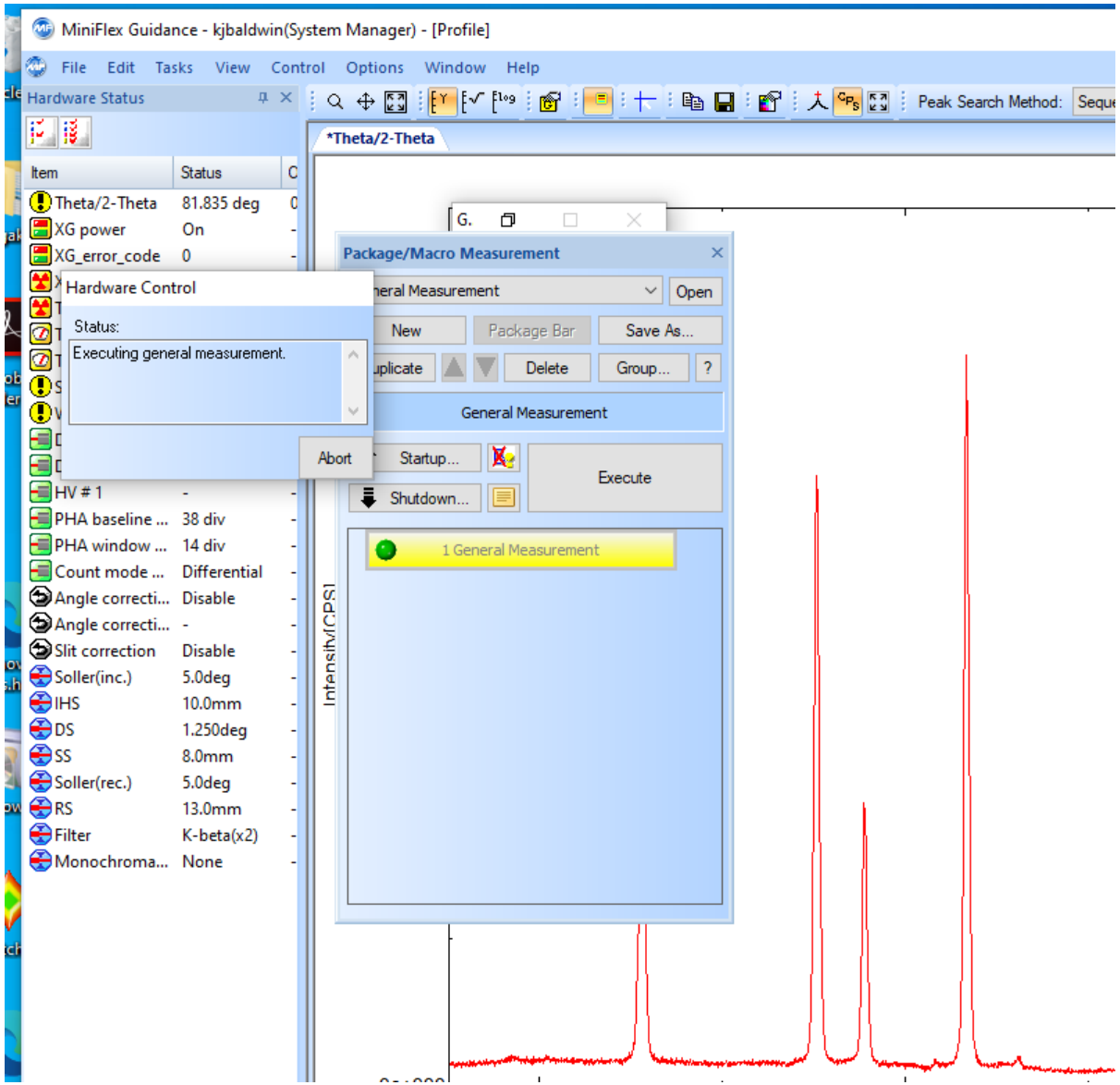
14 Load the sample.

14 General Measurement Click *Run.* A confirmation *Message* will pop up. Verify the information and click *OK*

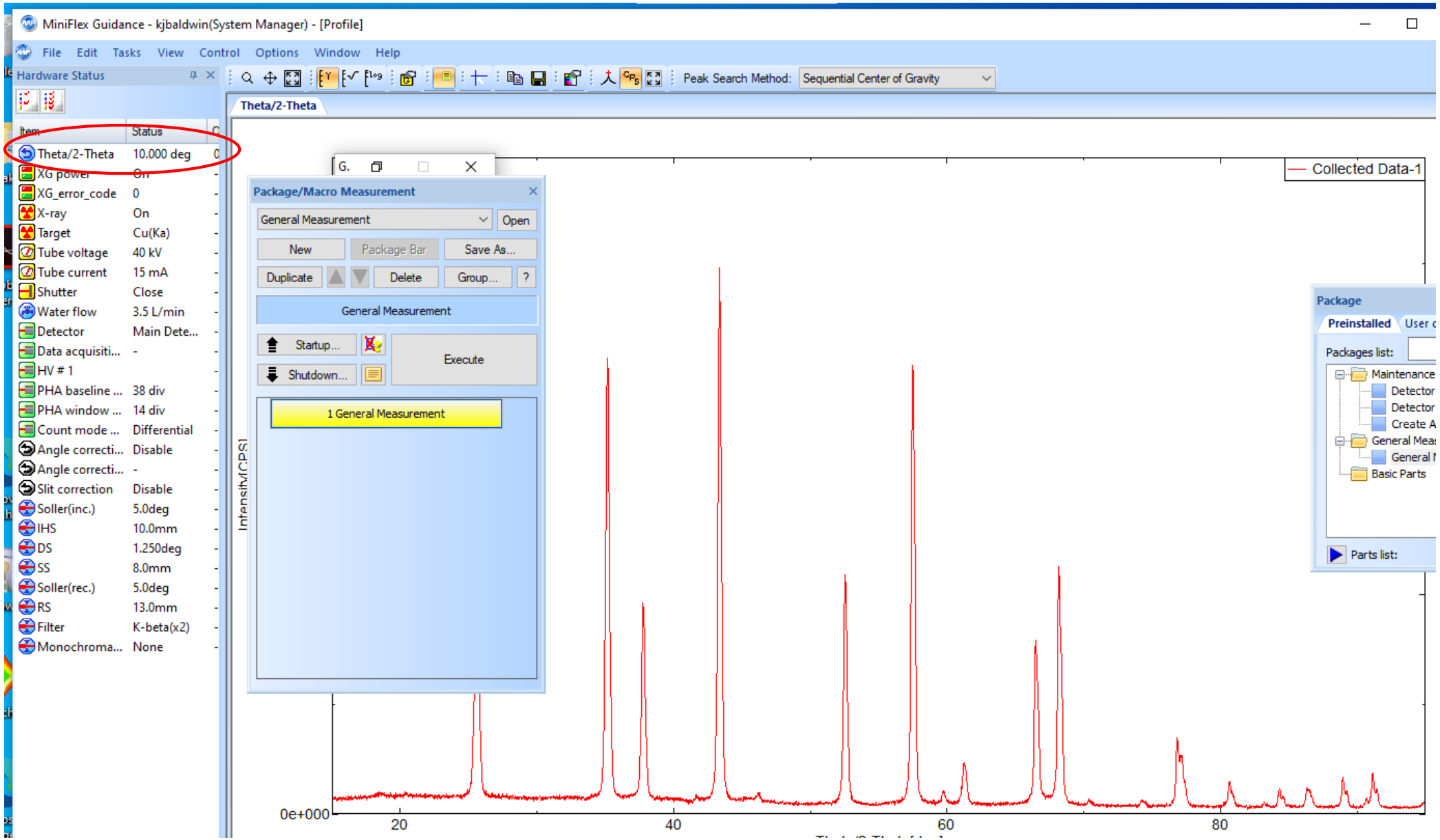




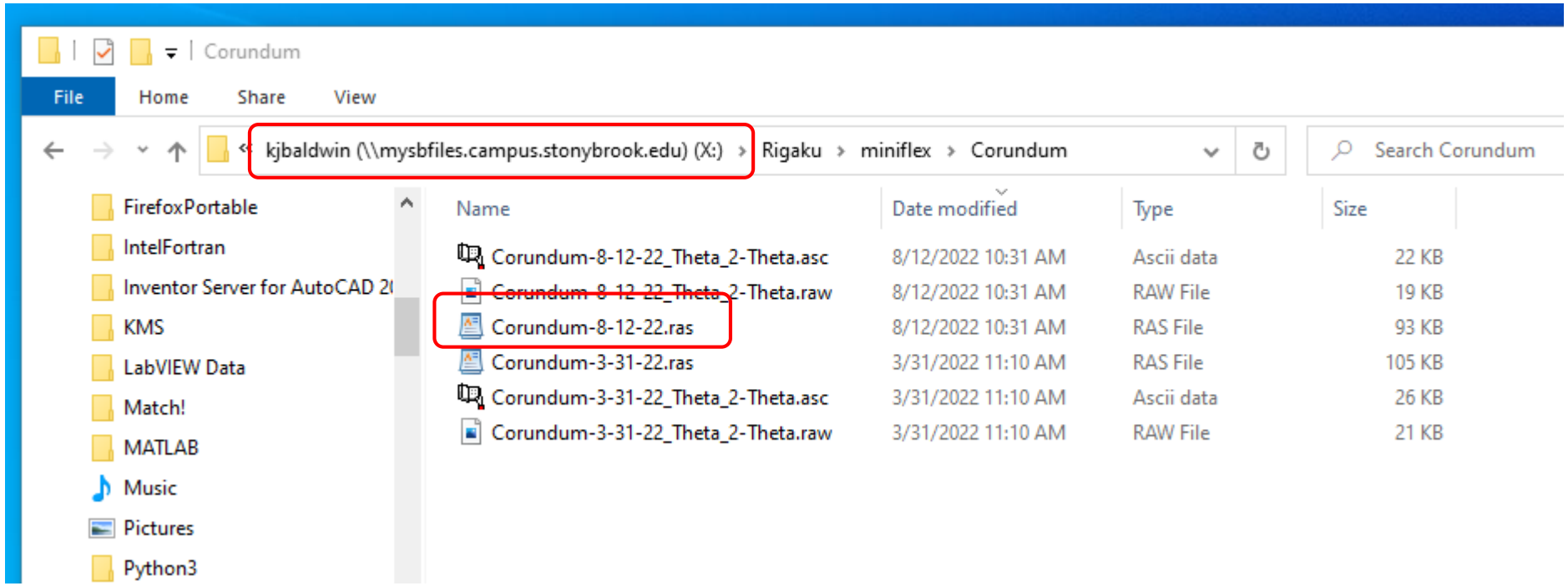
15 Data Collection in progress.



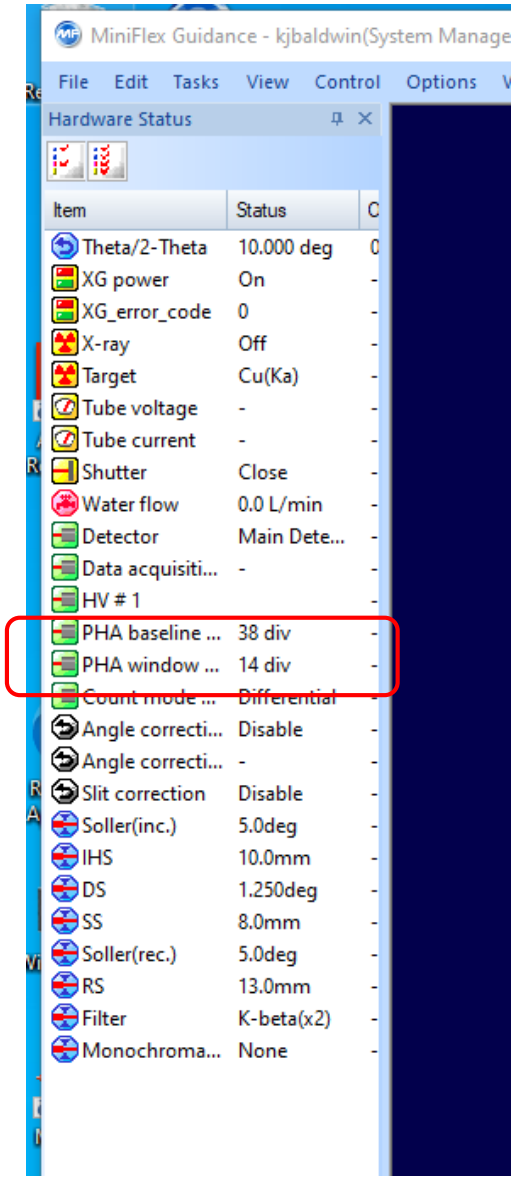
16a Data Collection finished. Notice that *Theta/2-Theta* is back to the home position, 10.000 deg.

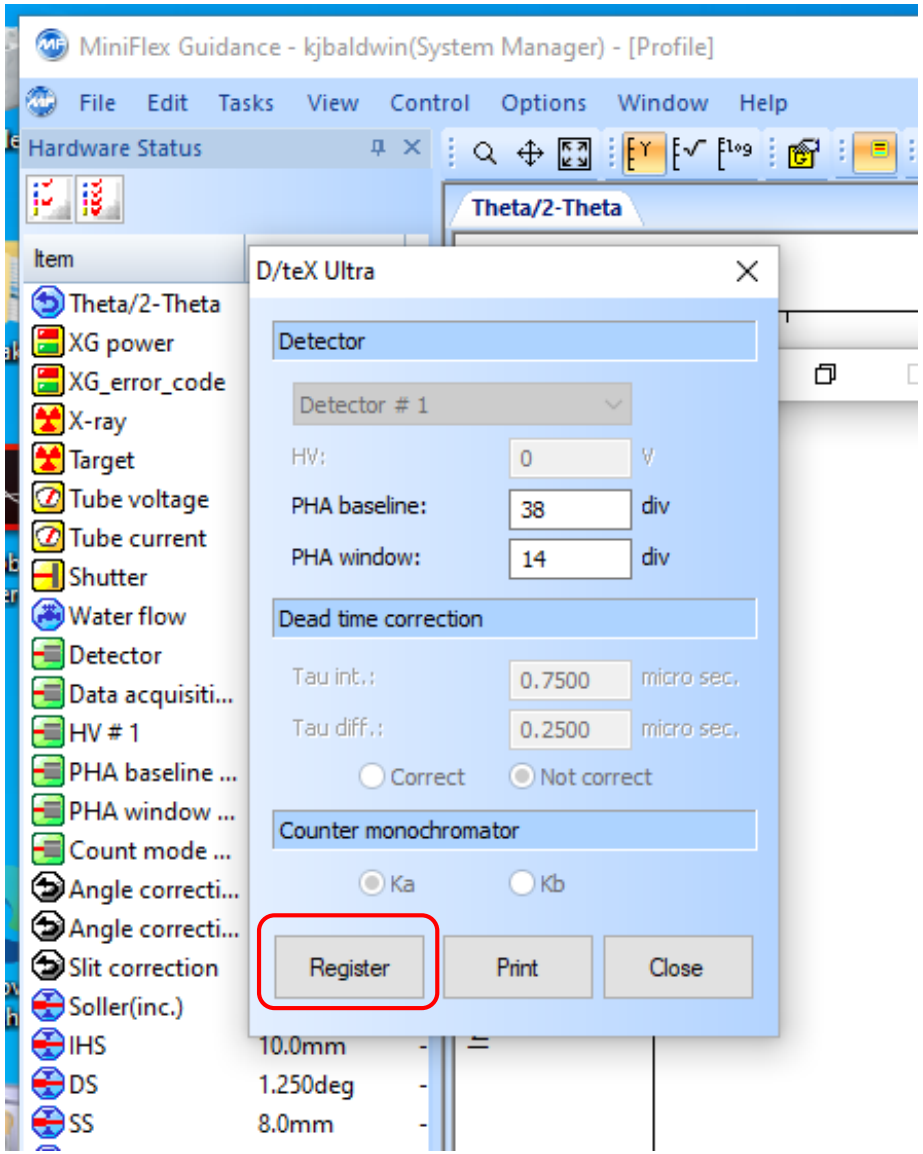


16b Data Collection finished. Open windows explorer and navigate to your *data directory*. Notice that three files have been created. *Corundum-8-12-22.ras* is file containing the raw data.



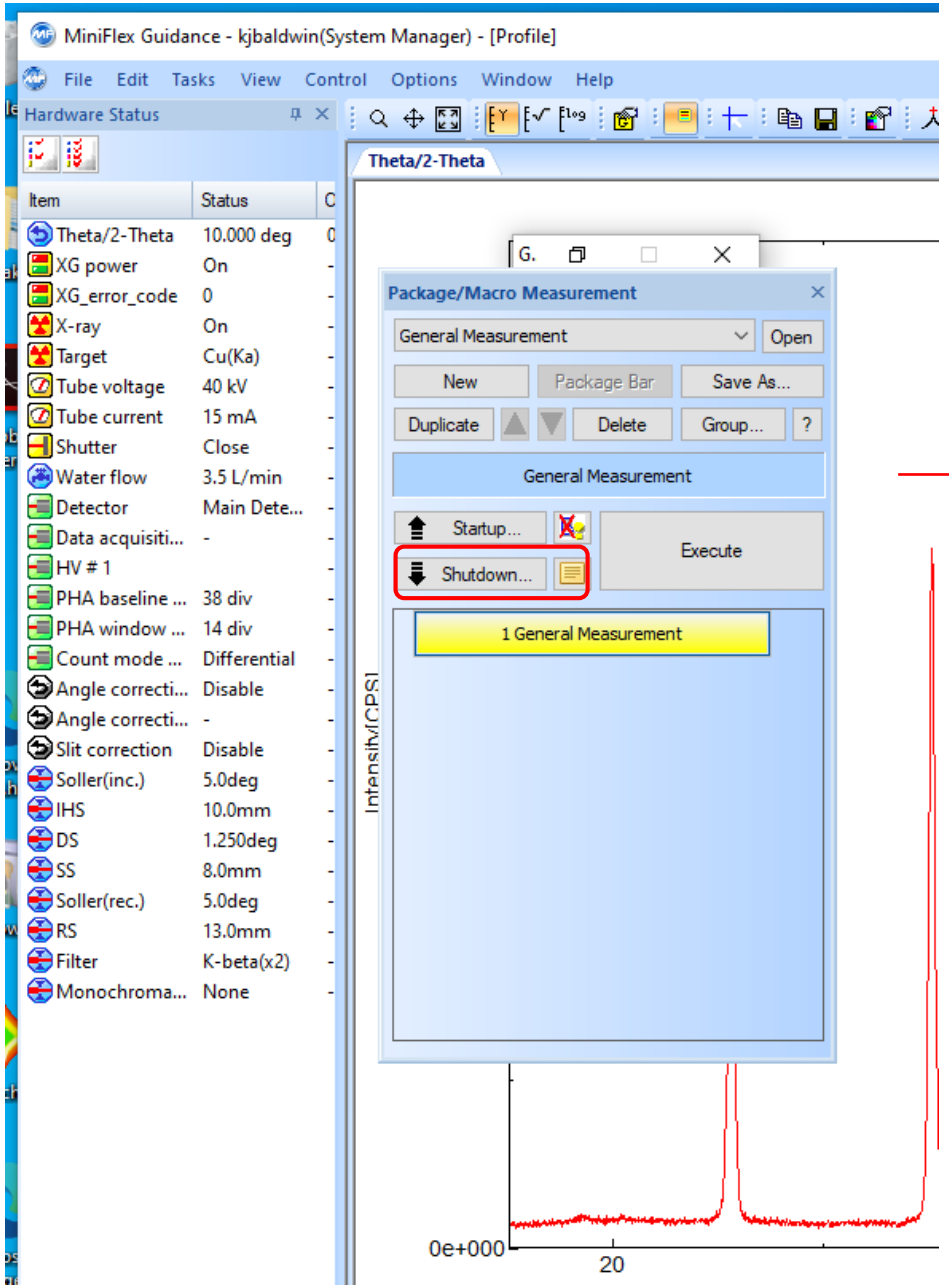
17a Adjusting the PHA to minimize Fe fluorescence. Adjust the PHA baseline and PHA window:
Select *Options →Detector Setup → 1 D/teX Ultra.* Enter the desired values and click *Register*

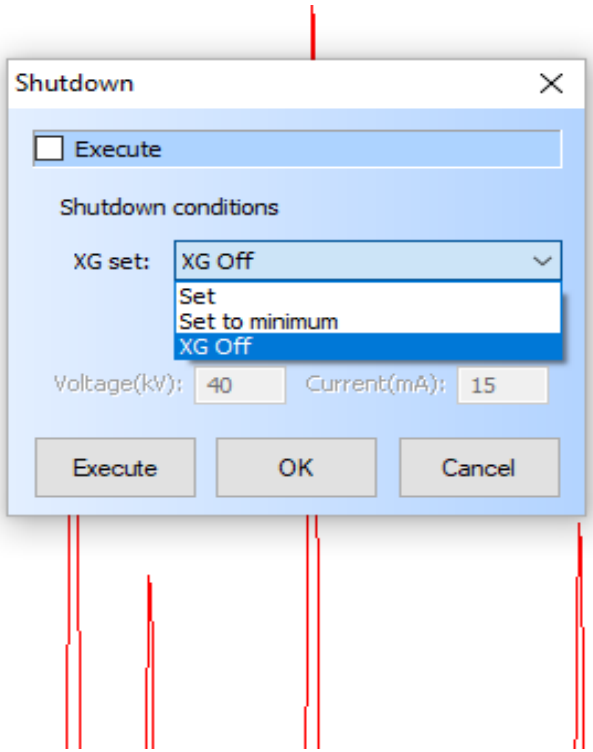


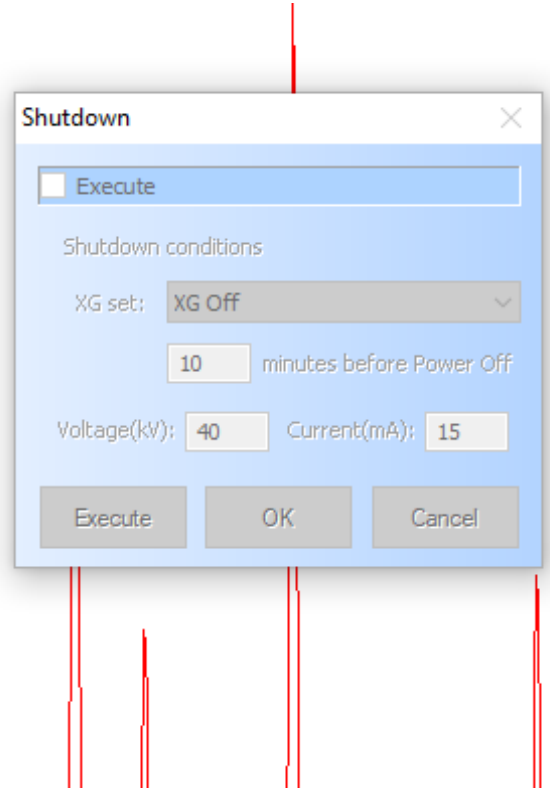


Mode	Baseline	Window
Normal	38	14
Fe	45	7

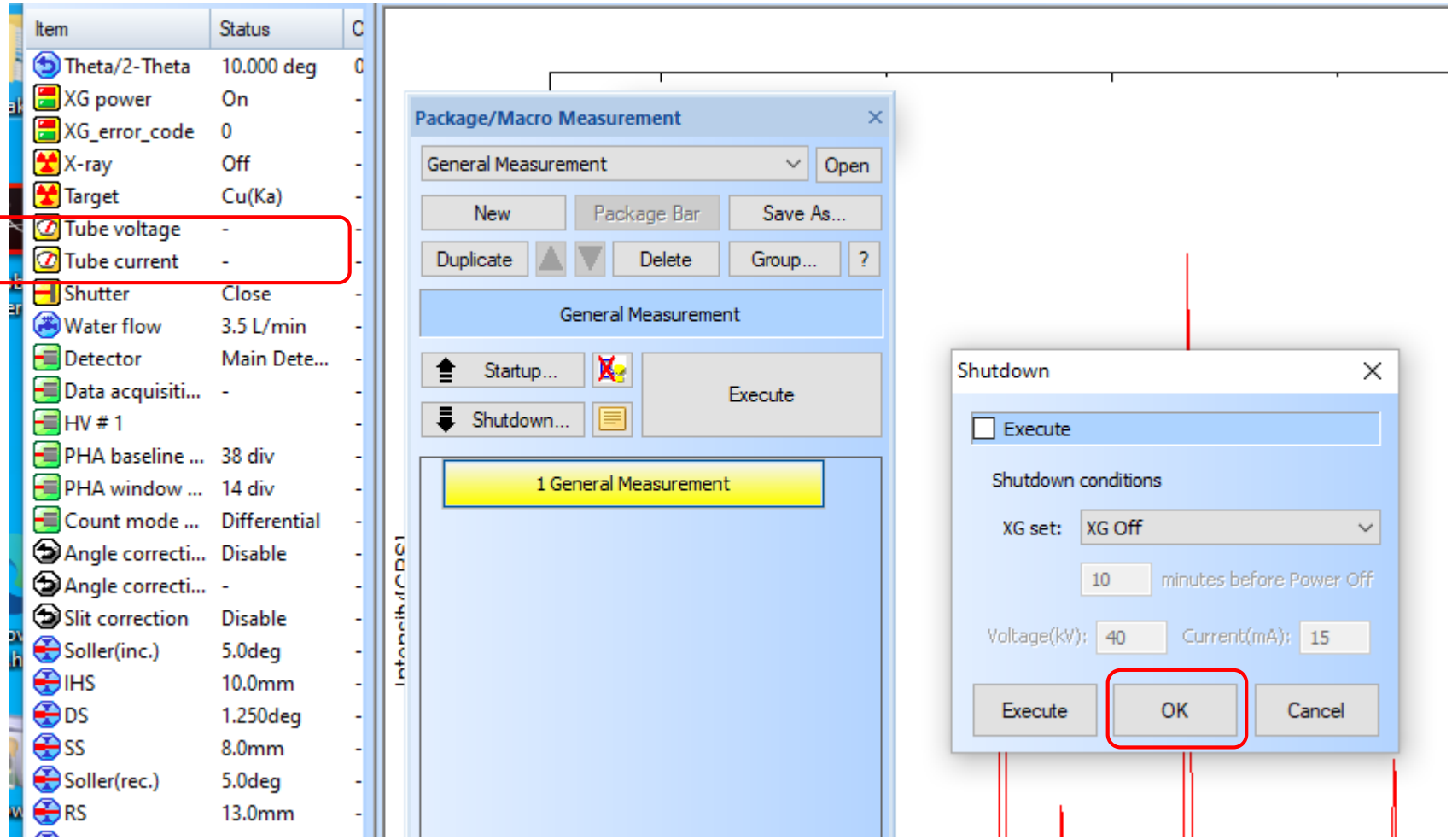
18a Turning off the generator. Click *Shutdown*. In *Shutdown* window select XG Off. Click Execute





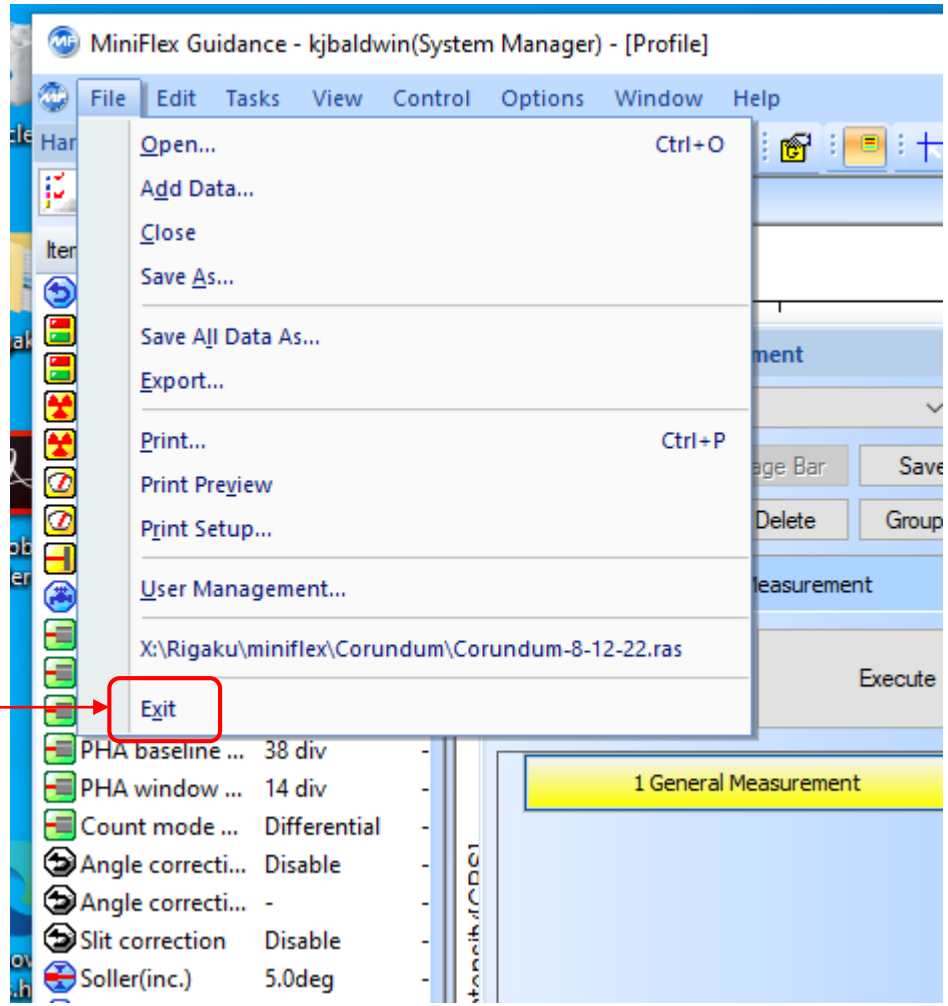


18b Turning off the generator. Once the generator is off the *Tube Voltage and Current* will be blank. In the *Shutdown* window click *OK.* Do not turn off the heat exchanger yet.



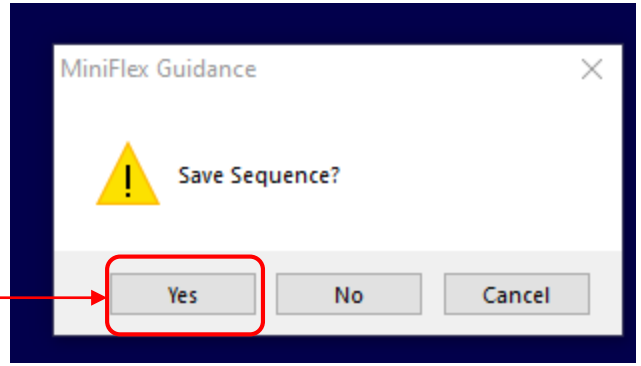
19a Exiting from MiniFlex Guidance.

From the File menu select *Exit*

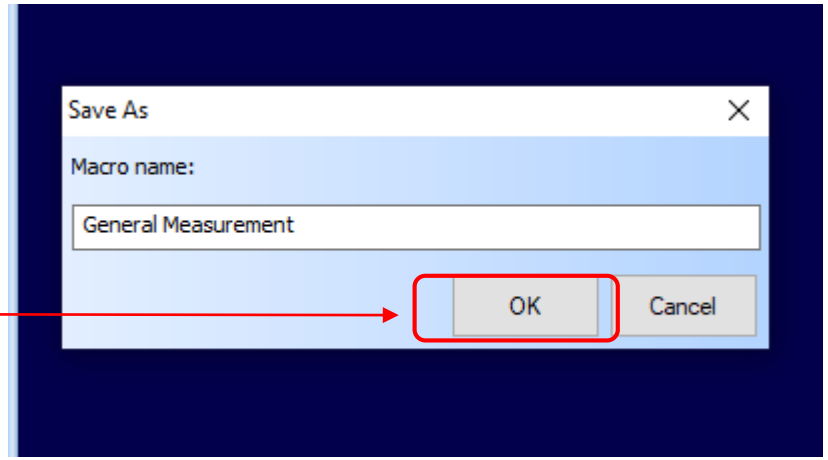


19b Exiting from MiniFlex Guidance continued. After selecting *File* → *Exit,* three message boxes will pop up .

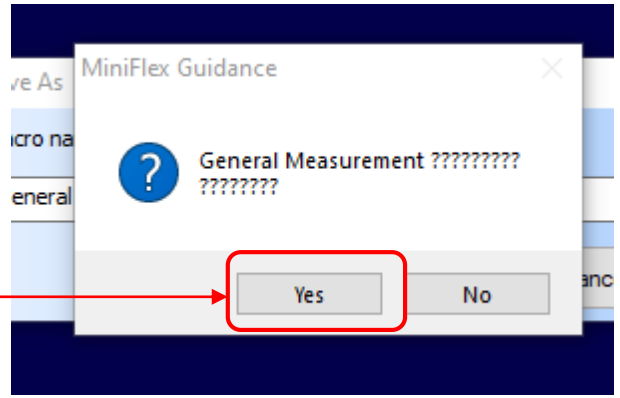
1. Click *Yes*



2. Click *OK*

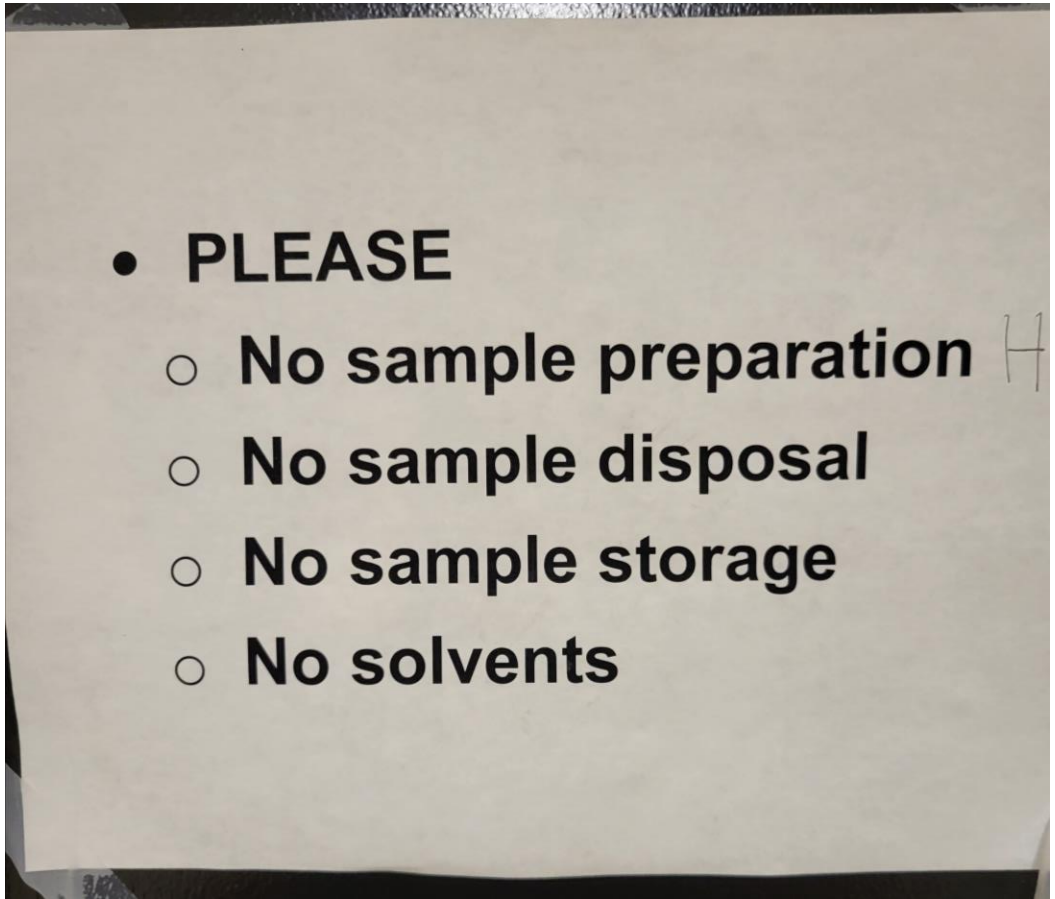


3. Click *Yes*



20 Finishing up.

1. Remove your sample.
2. Turn off the diffractometer. Refer to the first slide.
3. Finish filling out the log sheet. Please enter total time as decimal hours.
4. Turn of the Haskris heat exchanger.
5. Log of the computer. **Do not Switch user**, **Sign out**!
6. And finally



Using the Google Calendar to Reserve the Diffractometer

Step 1. Add the Resource Calendar to your Google Calendar.

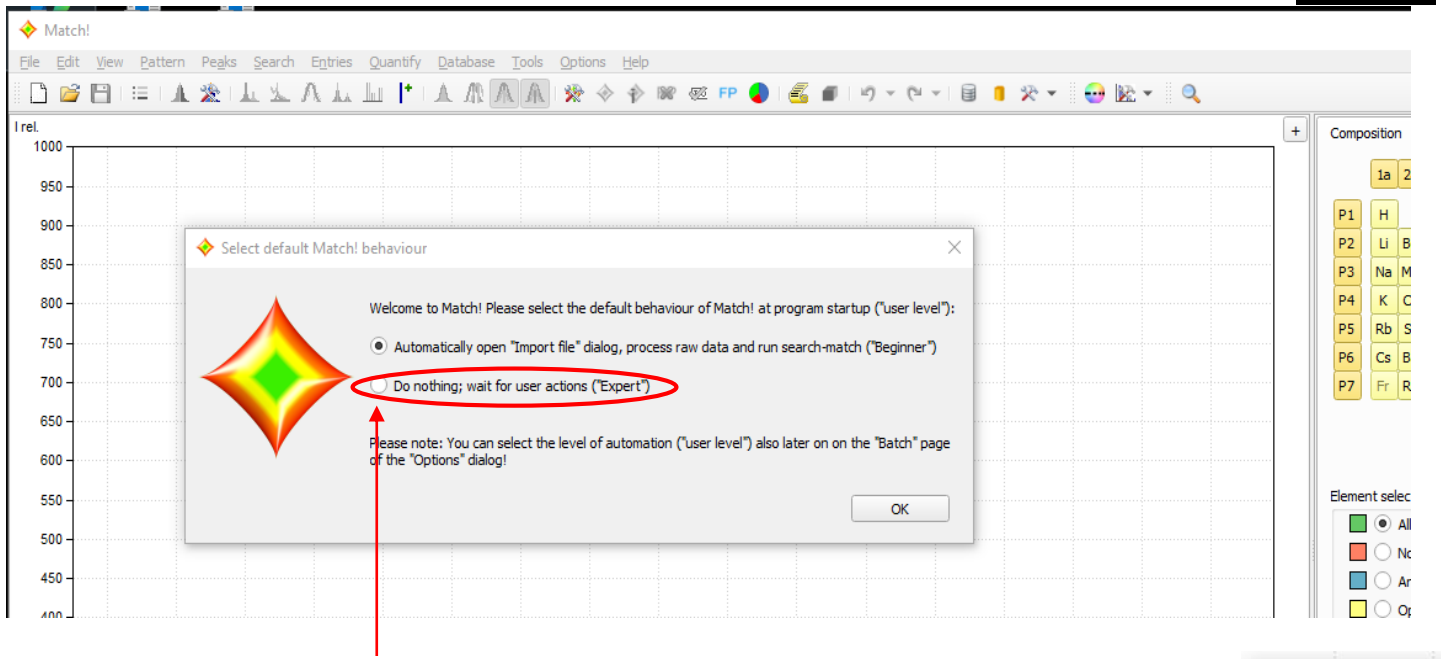
- Open your Google Calendar and scroll down the left side information until you come to "Other calendars". Click on the + symbol.
- Click on "Browse resources"
- Scroll down through the A-Z named resources until you come to "(Room)" and click on that.
- Check the box for ESS-GEO Room-245-25
- Return to your calendar
- You can make the ESS-GEO Room-245-25 calendar display on your calendar or not by giving it a distinct color and checking or unchecking the box next to it. When it is displayed, you should be able to see the details of existing reservations.

Step 2. Reserve the diffractometer

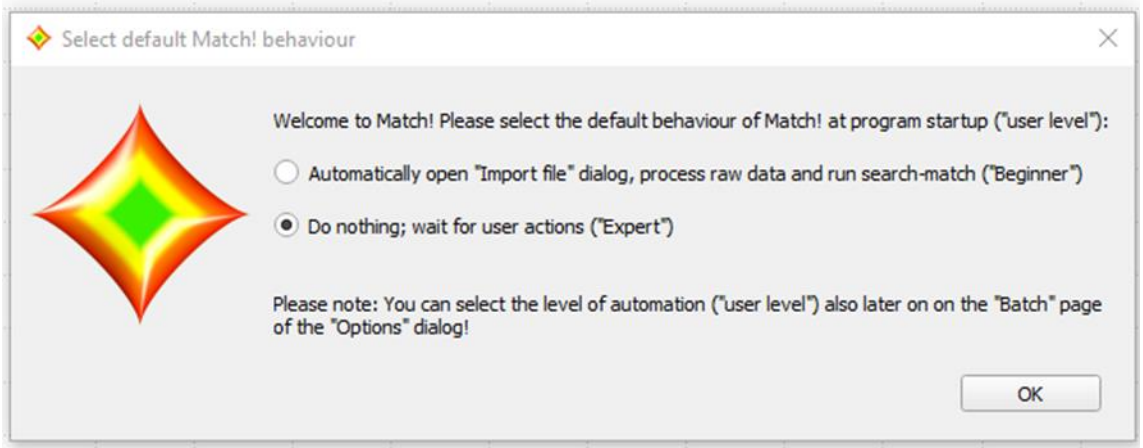
- Select a day/time in your Google Calendar giving it a title that includes ‘XRD’, your name and email address.
- Select the "Rooms" tab on the right hand side next to "Guests".
- In the search box below "Rooms", start to type "ESS-GEO" and you will see the resource calendar for ESS 245 show up in the results.
- Select the ESS-GEO Room-245 resource and save.

Using **Match!** to Reformat Diffraction Data

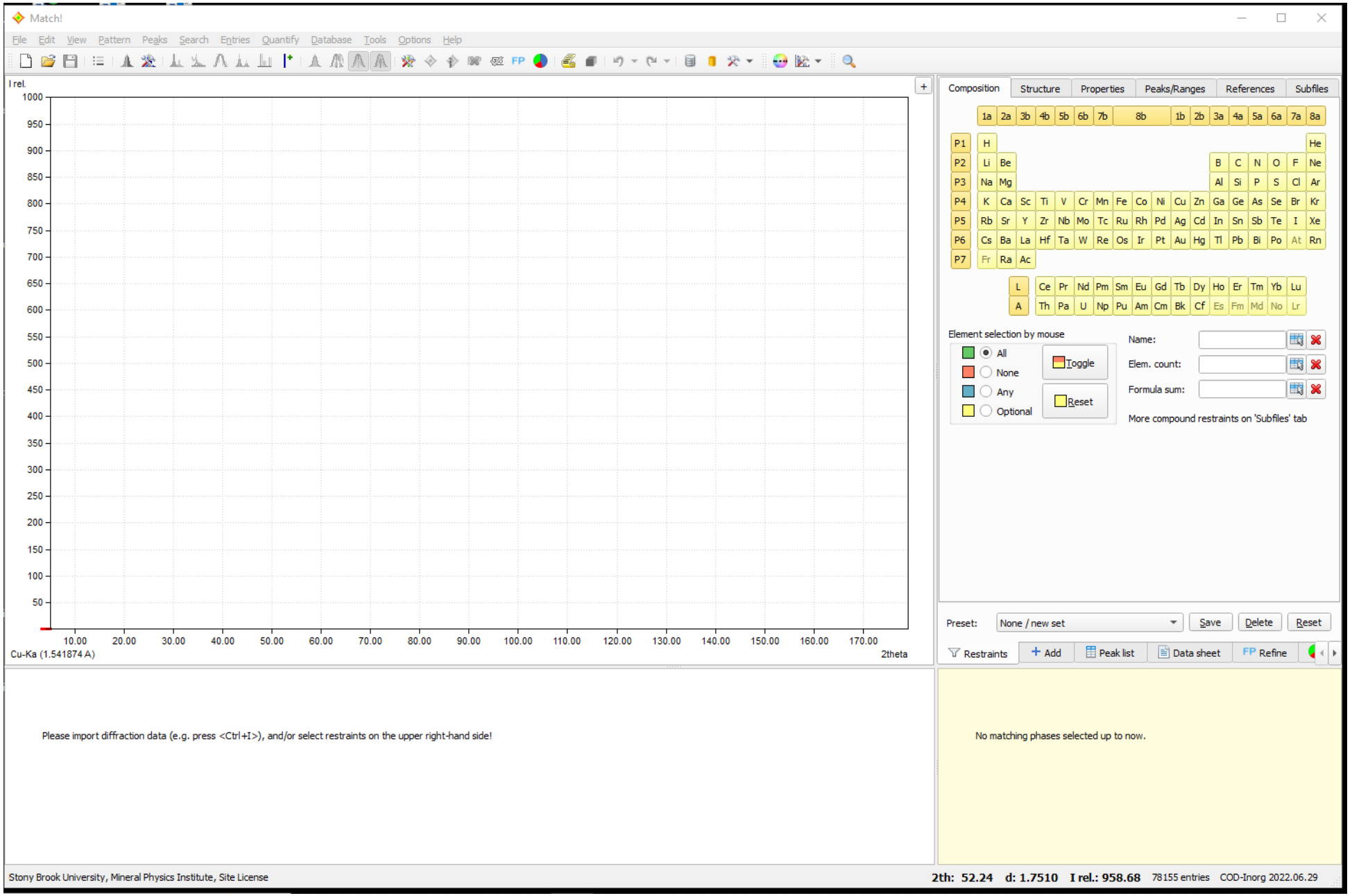
Step 1a. Start Match! by double clicking the desktop icon.



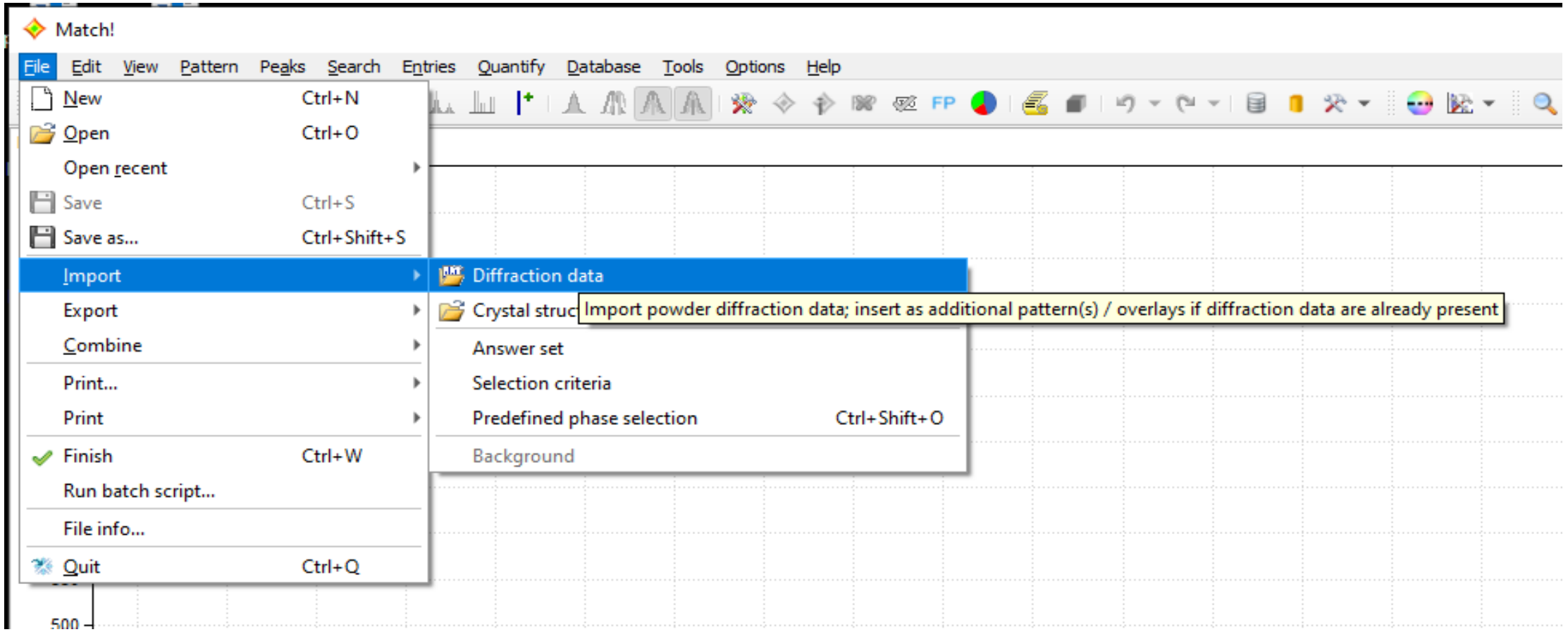
Step 1b. Click on *Do nothing; wait for user actions ("Expert")*



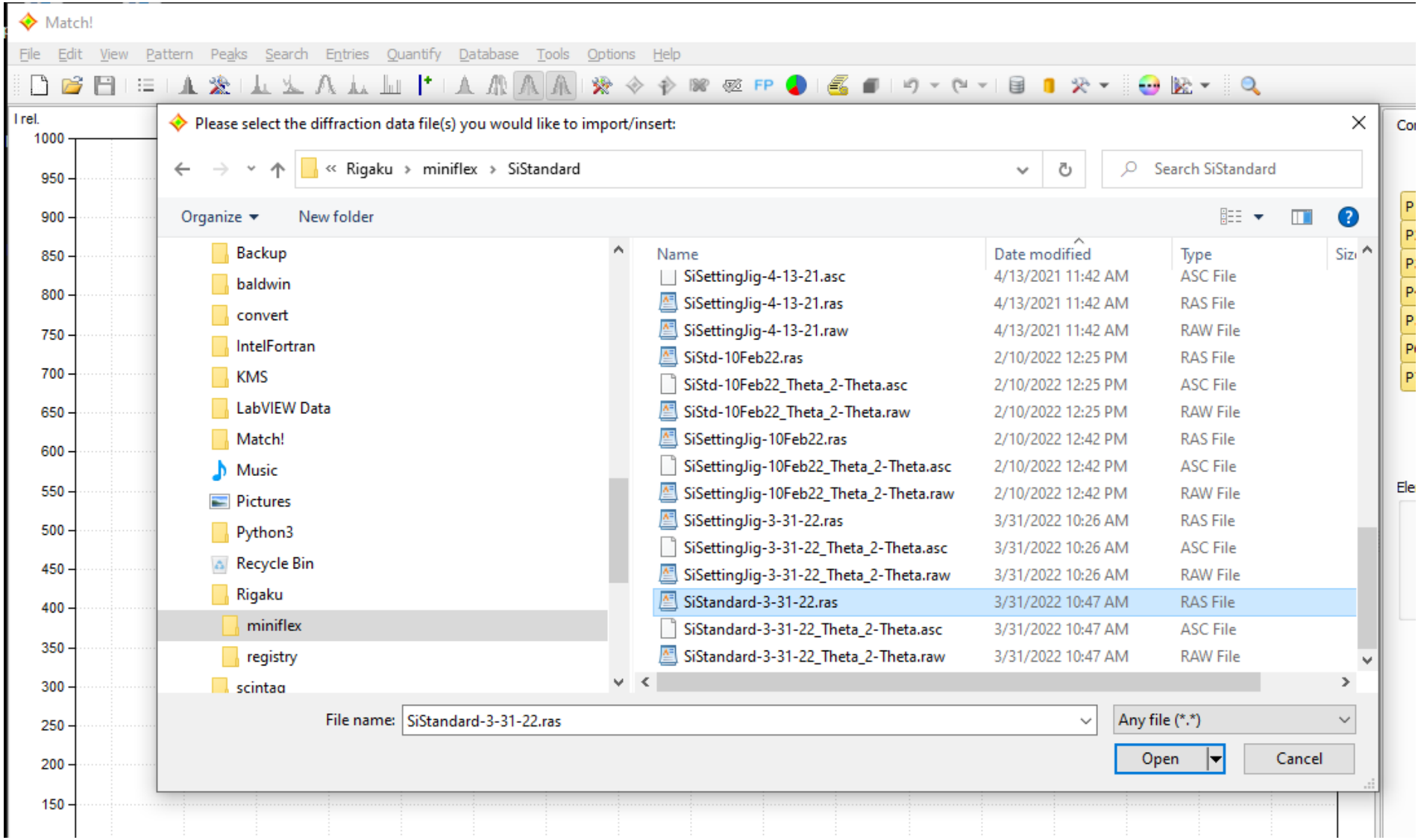
The Match! program is now loaded and ready.



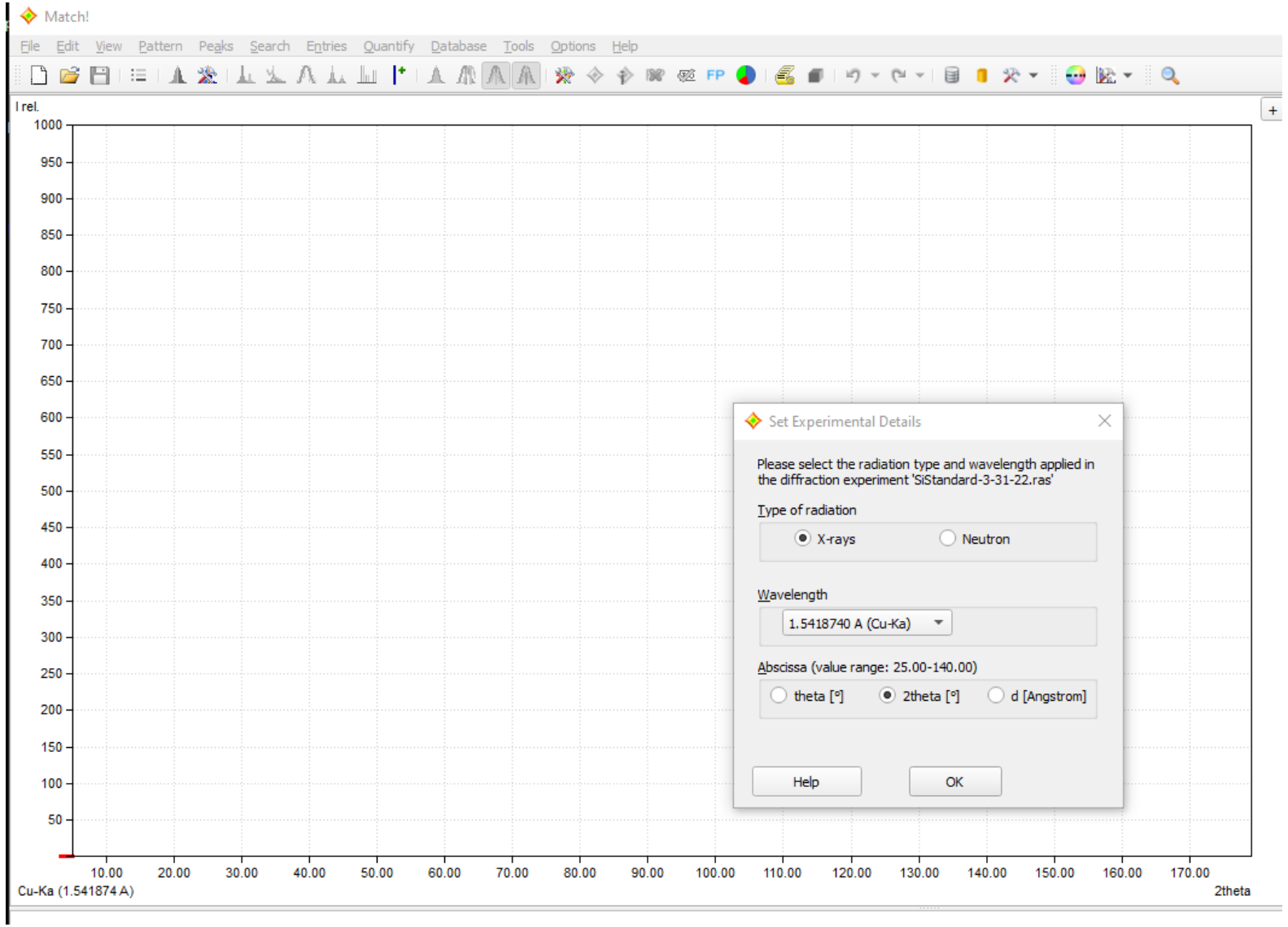
Step 2. Select *File* → *Import* → *Diffraction data*



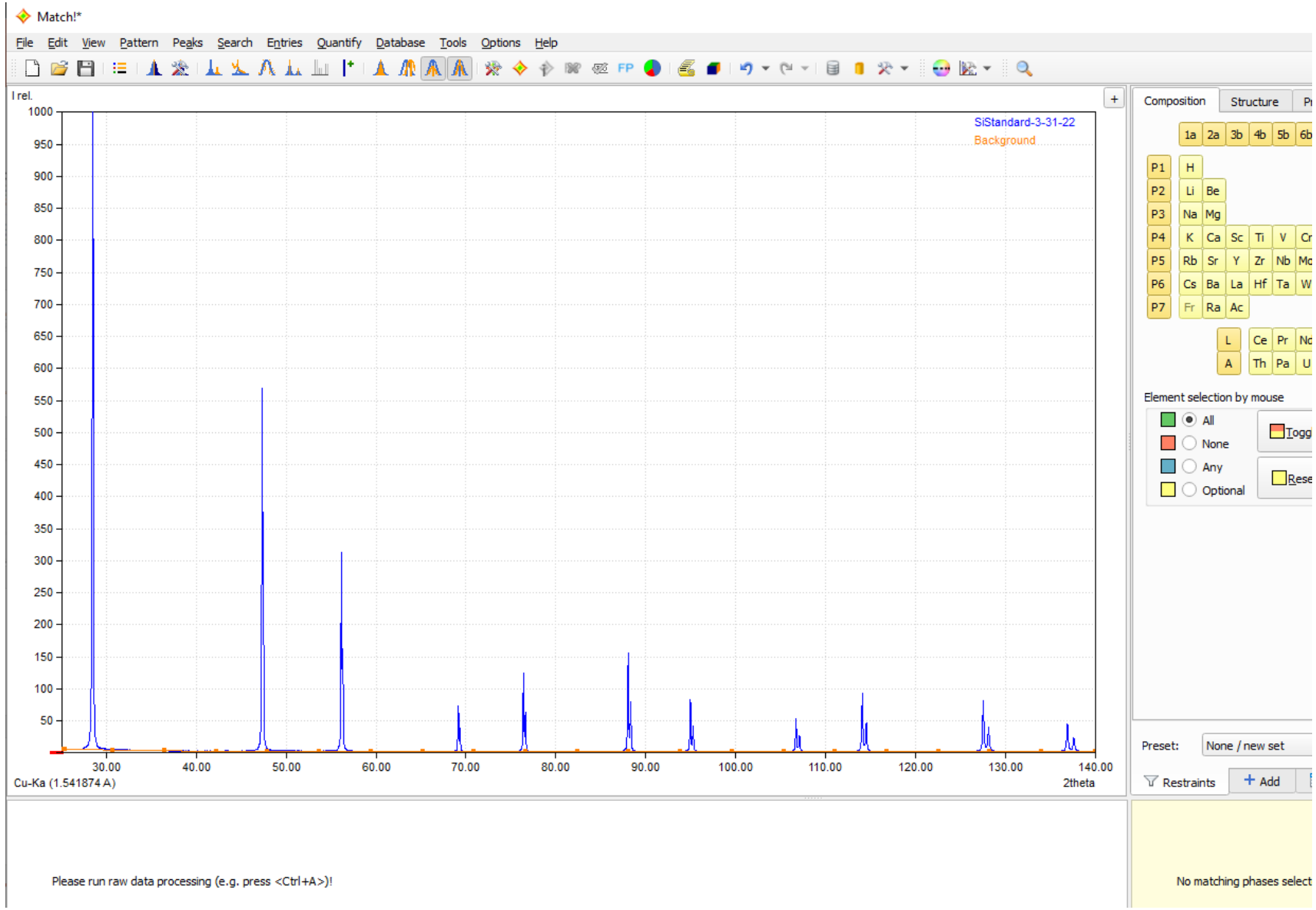
Step 2b. Select your datafile. Choose the file with the extension *ras*.



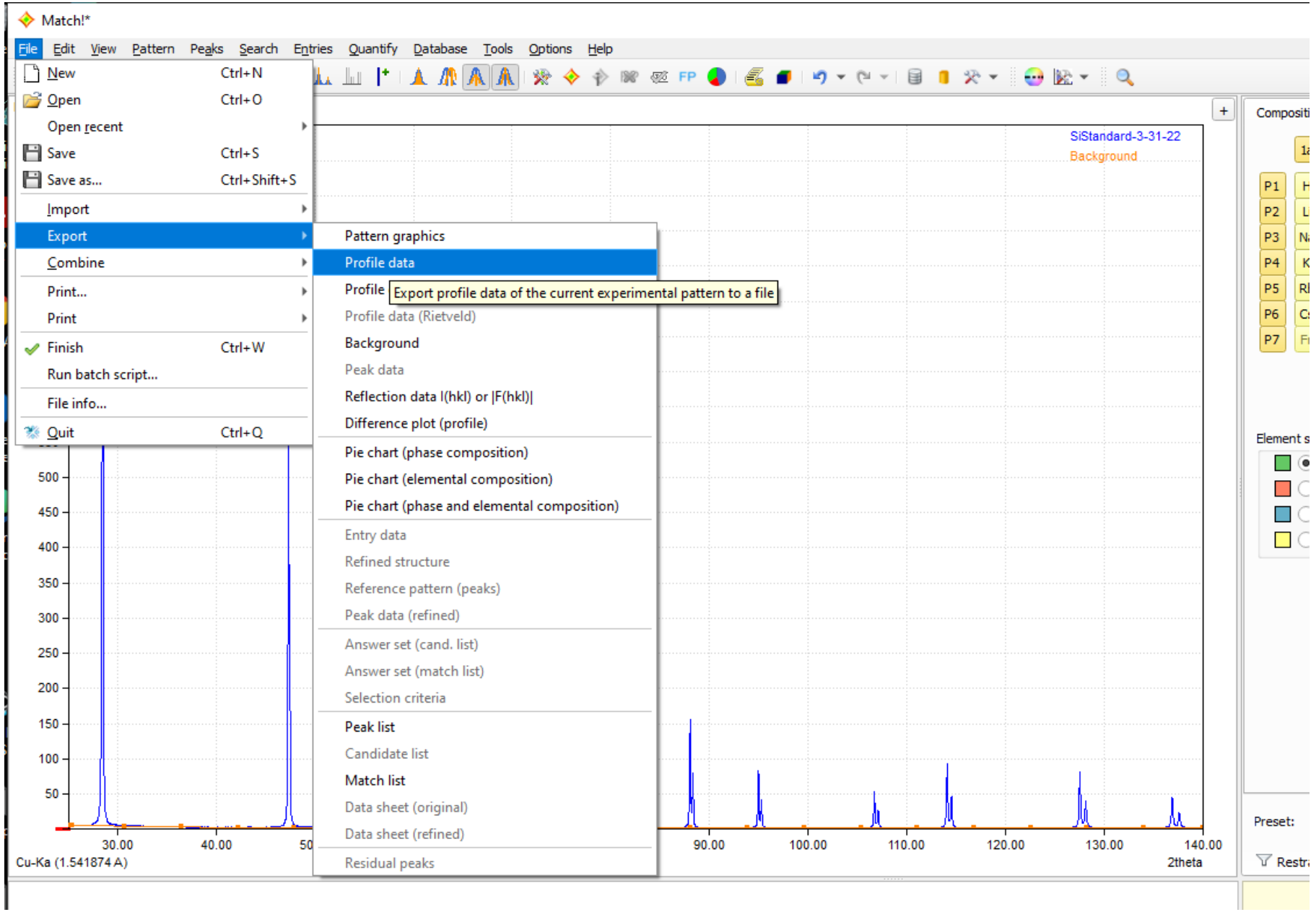
Step 2c When the window *Set Experimental Details* appears, click *OK*



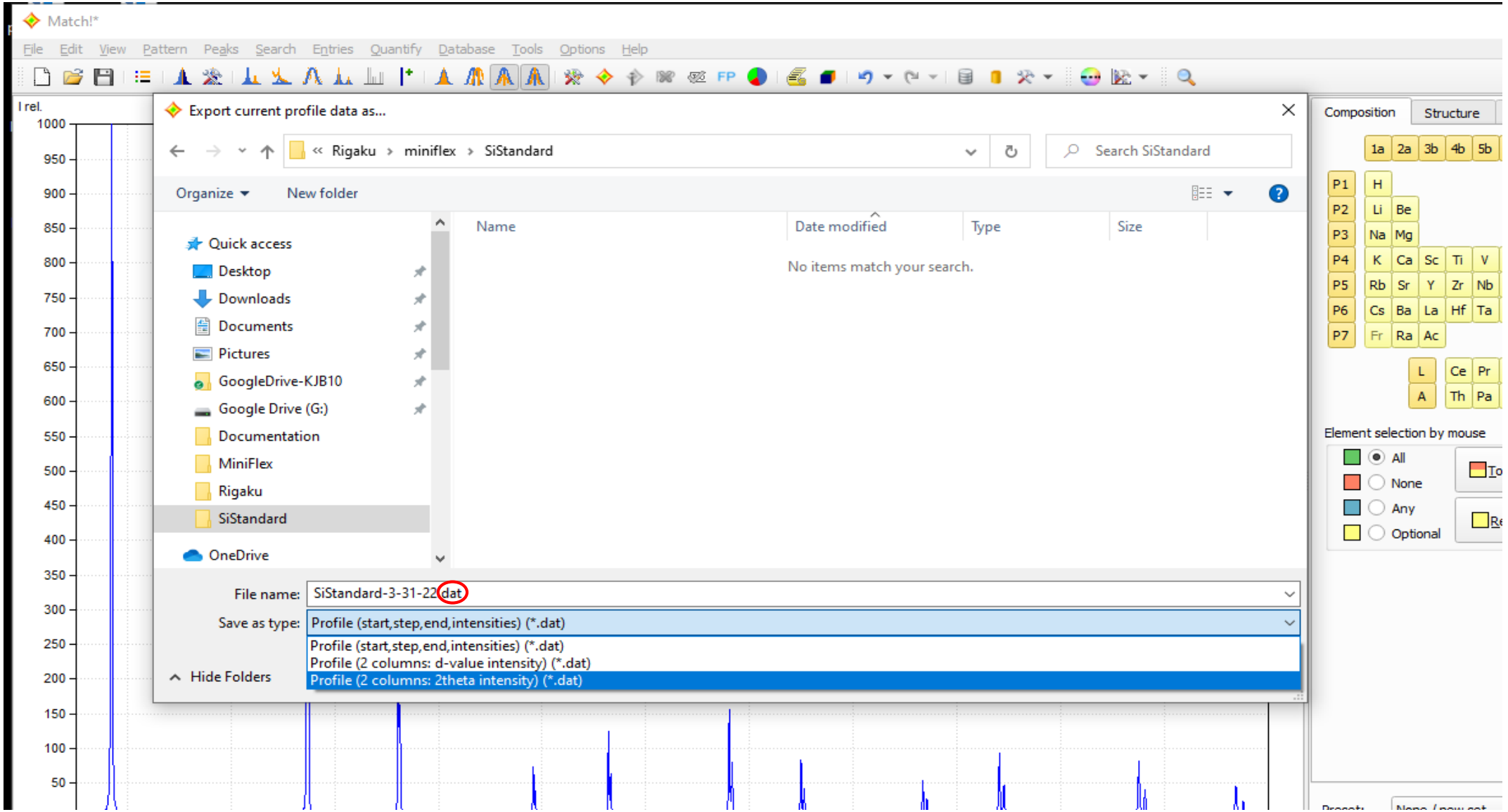
Your diffraction pattern will be displayed.



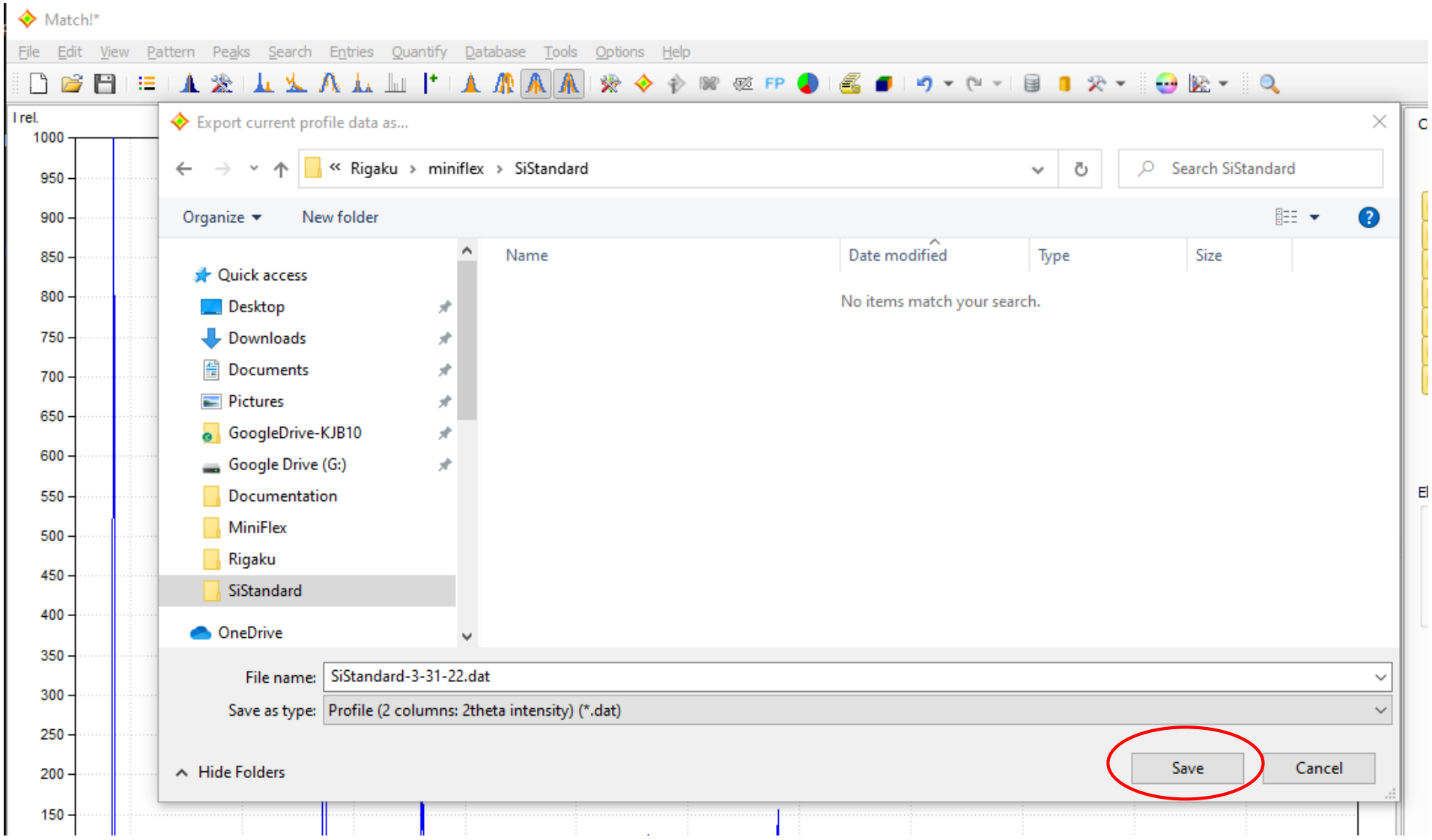
Step 3a. Select *File* → *Export* → *Profile data*



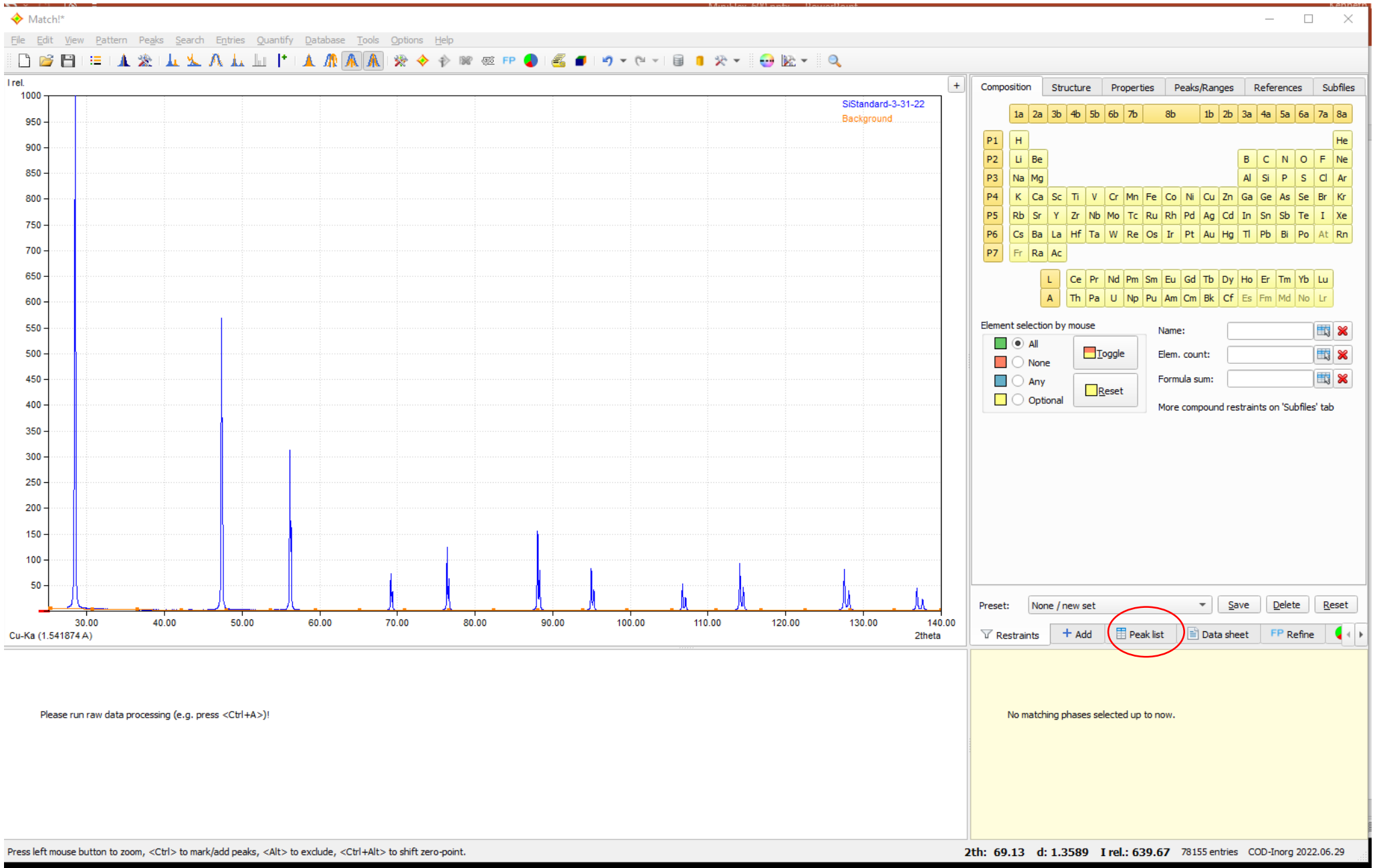
Step 3b. For *Save as type* Select *Profile(2 columns: 2theta intensity) (*.dat)*
If need be, you can change the extension *dat* to something else.



Step 3b Continued Click *Save*

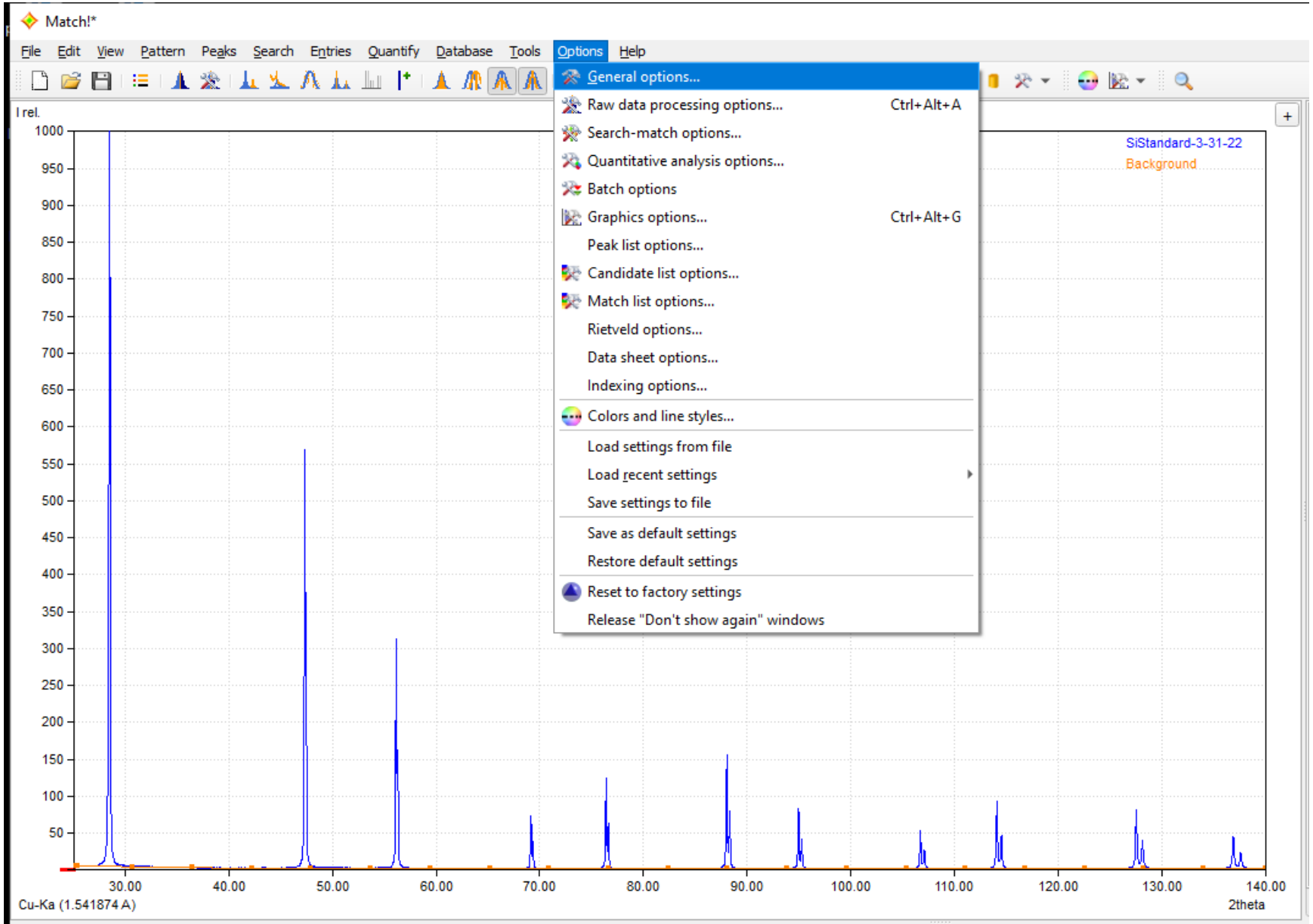


Match! Continued: Preliminary data analysis

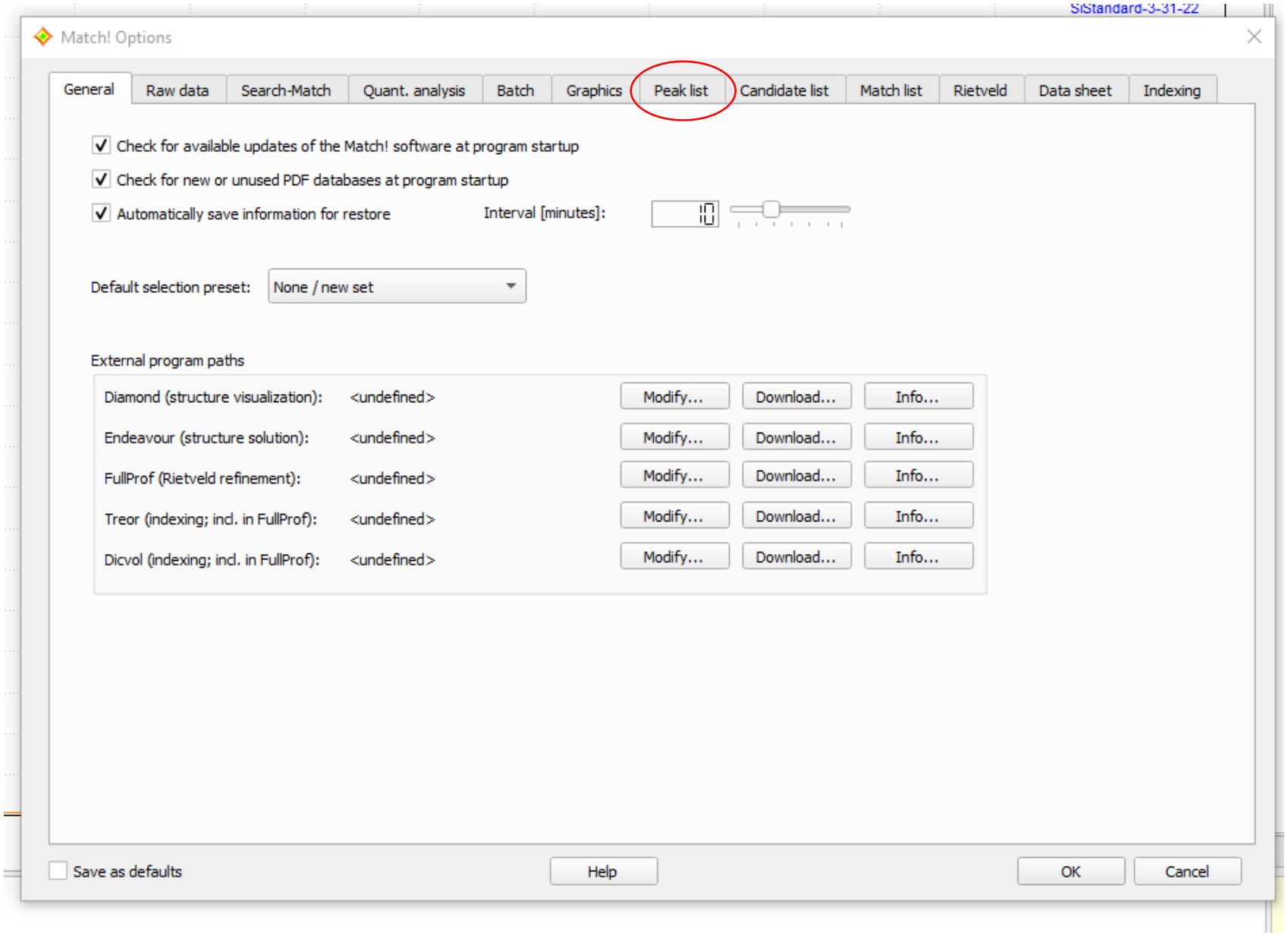


1.Click *Peak List*

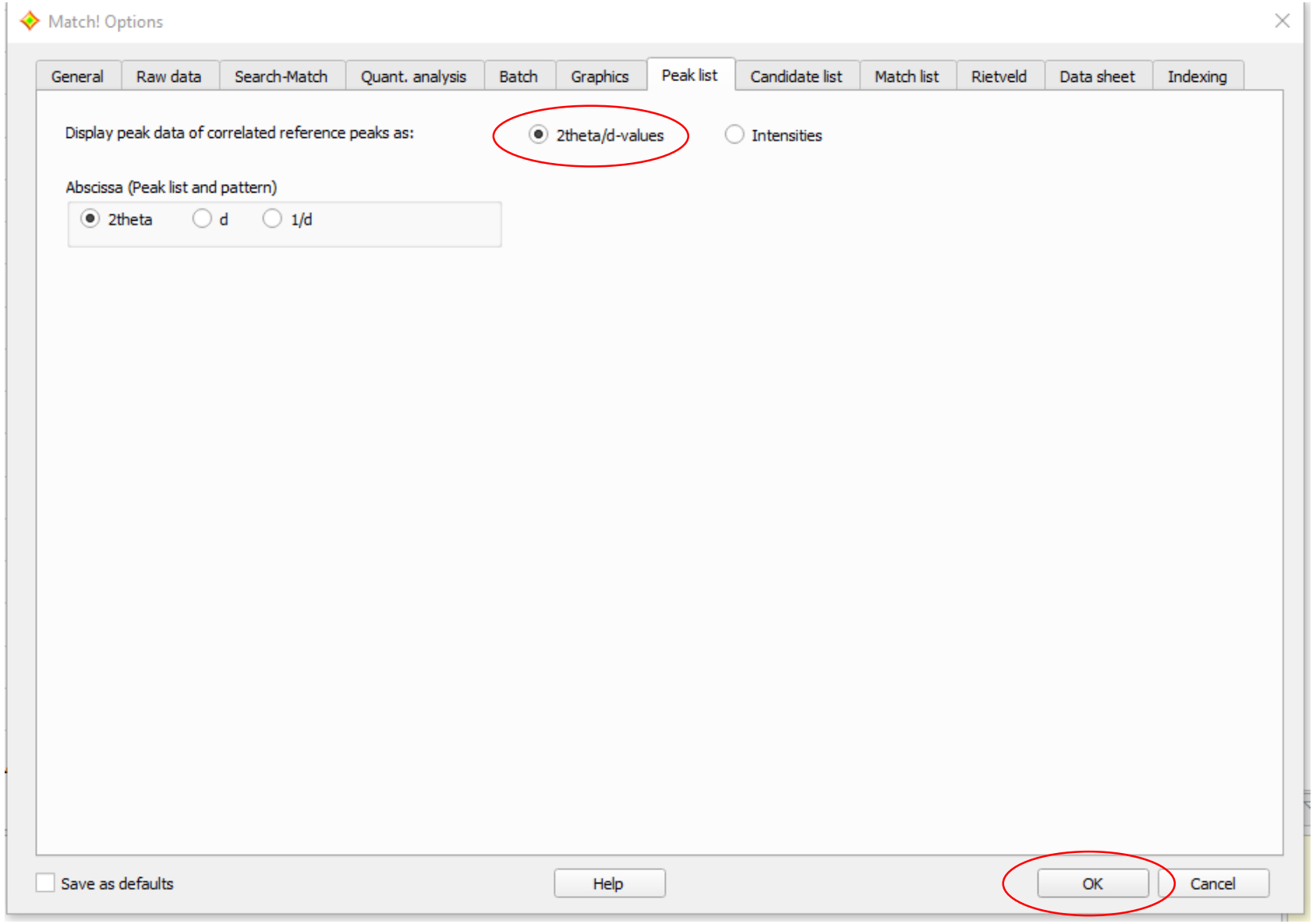
2. Click *Options* → *General options*



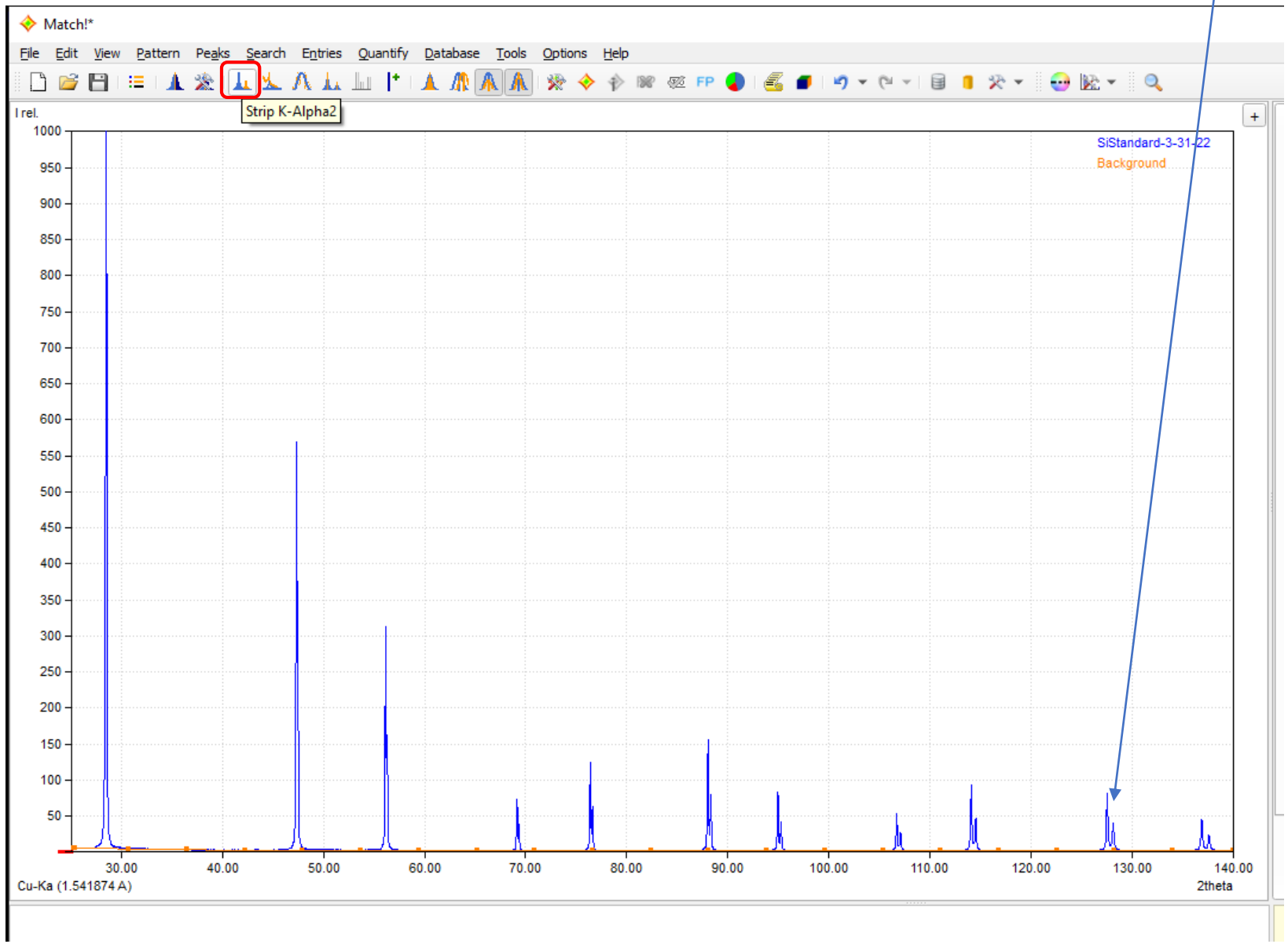
3. Click *Peak list*



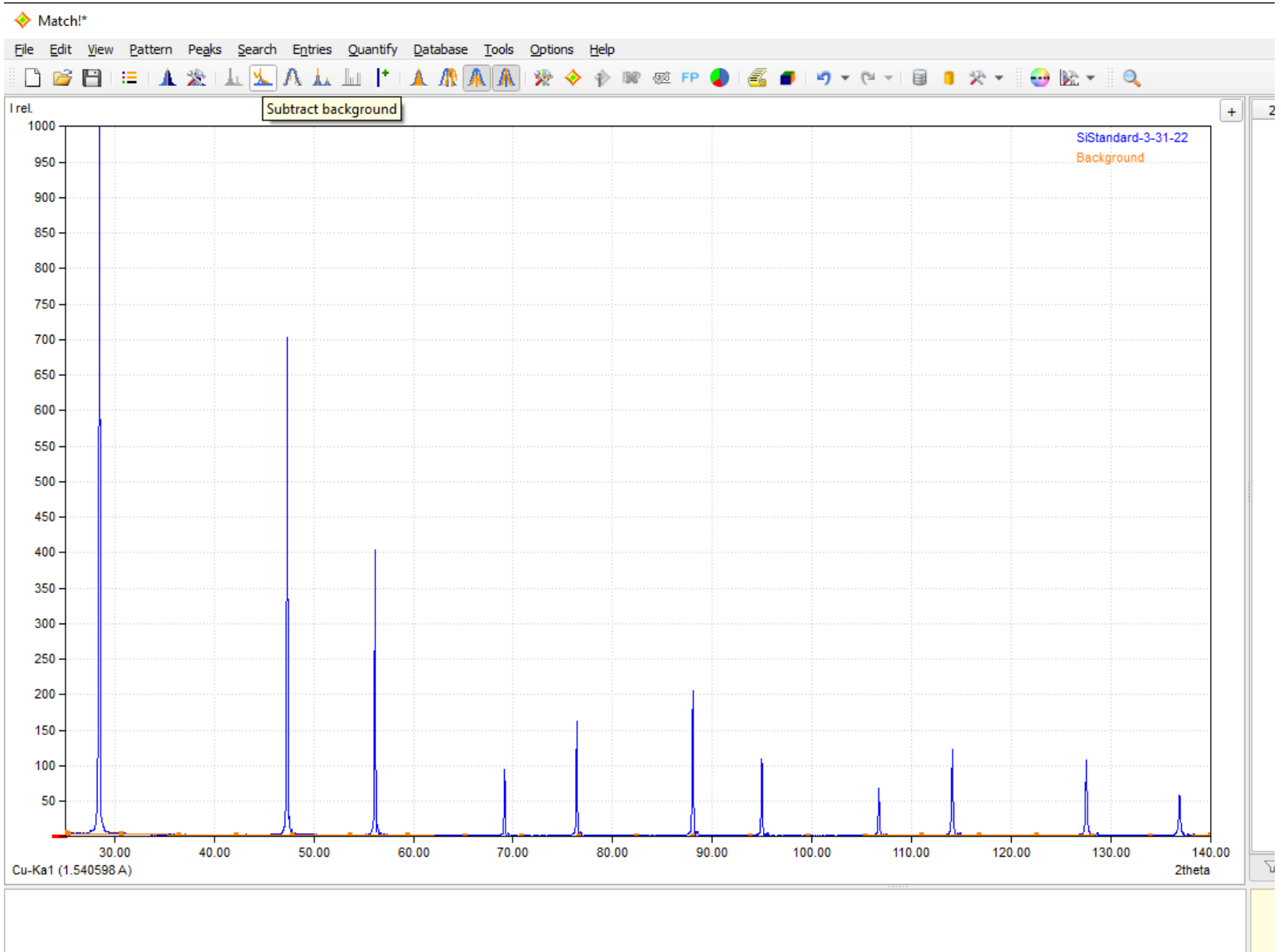
4. Select *2Theta/d-values* then click *OK*



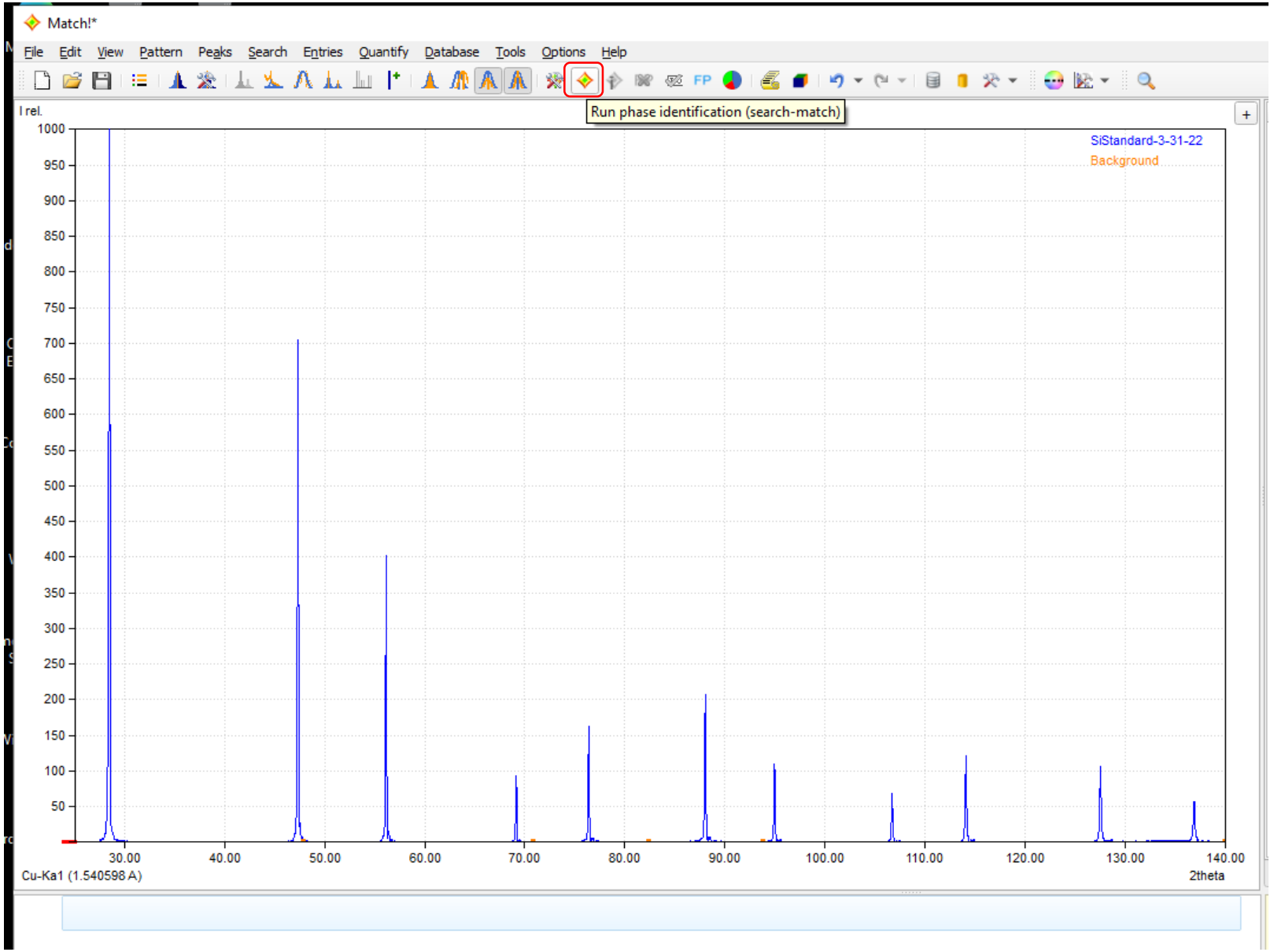
5. Click Icon for *Strip K-Alpha2.* Notice changes in the diffraction pattern. Like here.



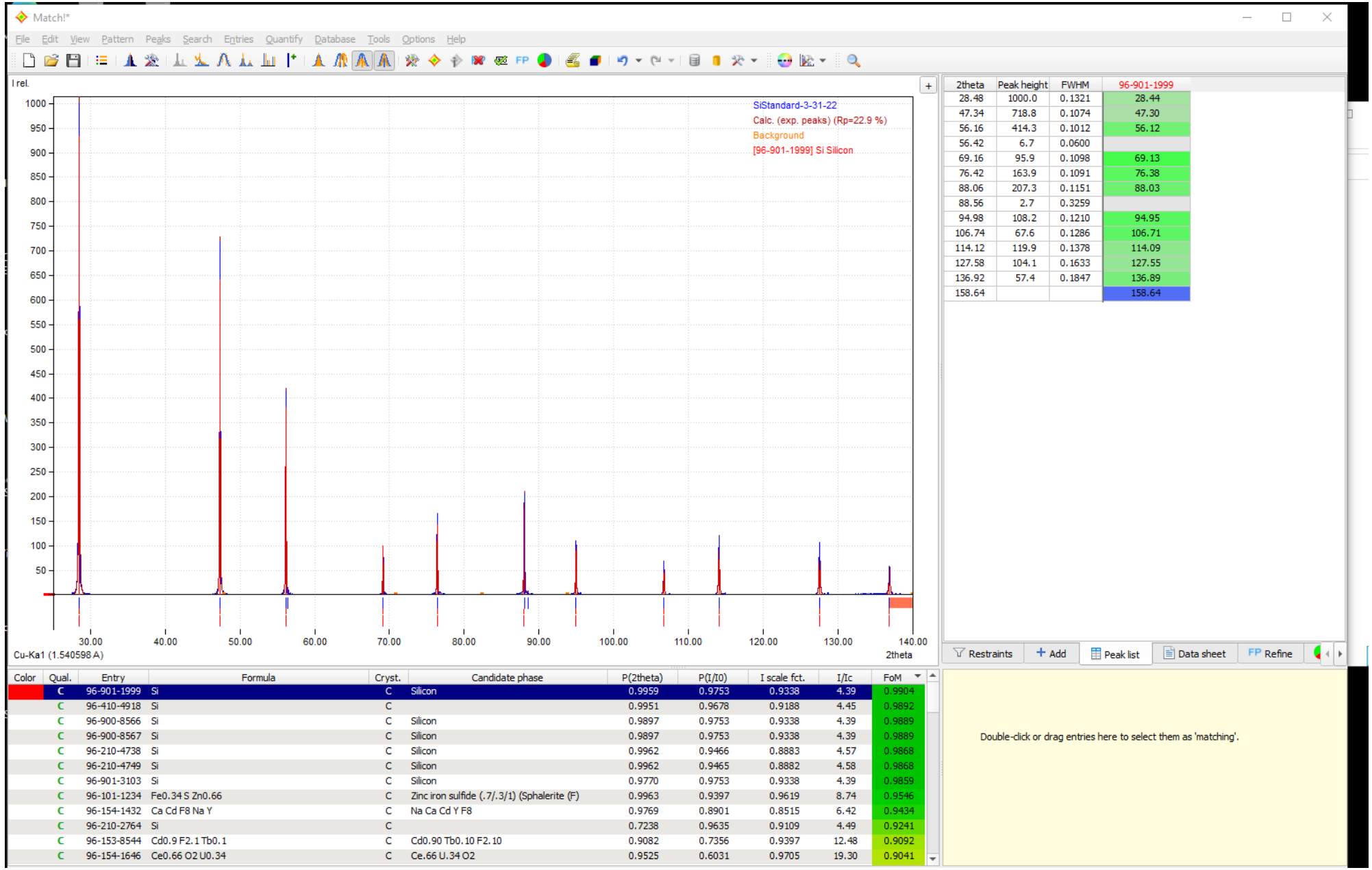
6. Click *Subtract background* and look for changes in pattern again



7. Click on Icon for *Run phase identification (search-match)*

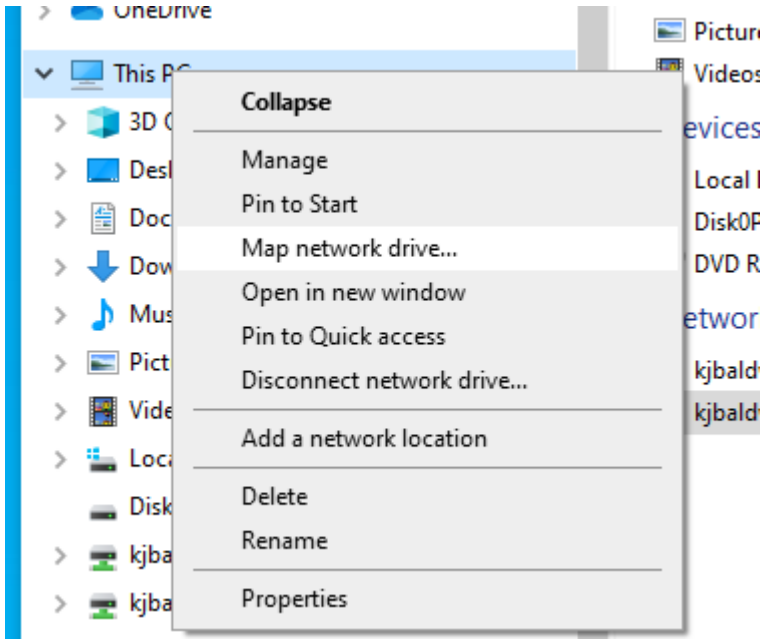


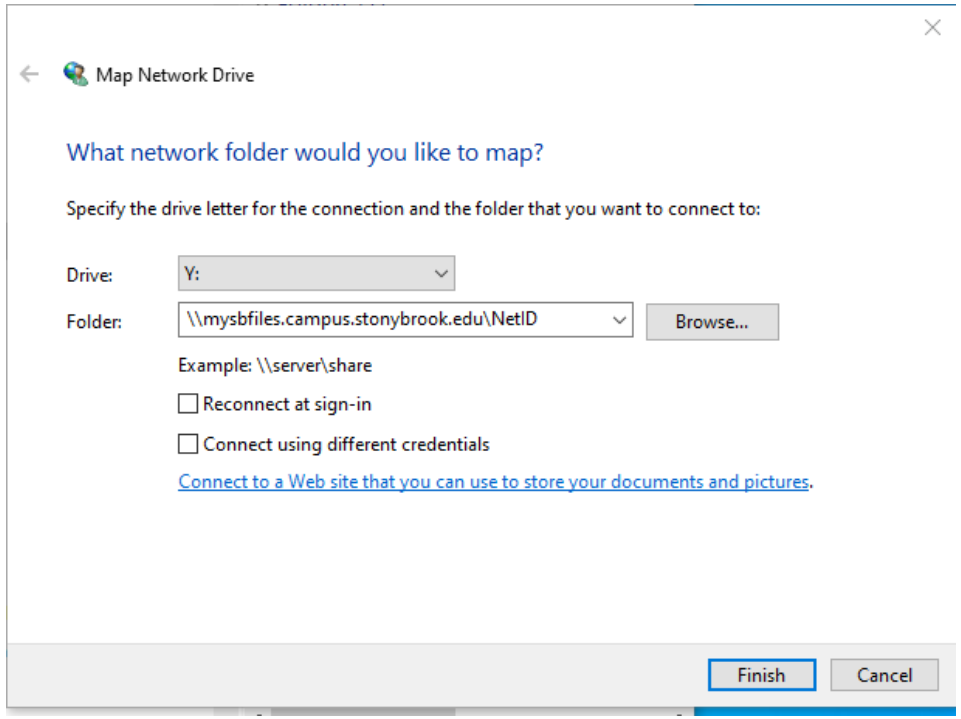
8. Observe Peak list



Manually mapping to your '*mysbfiles*'

1. Open File Explorer and right click on *This PC* and select *Map network drive…*





2. Select a *Drive letter* and the *Folder*: \\mysbfiles.campus.stonybrook.edu*NetID*
   Be sure to replace NetID with your actual NetID.
   Click *Finish*