Irena/PeakTool Manual
PeakTool v. 0.18

PeakTool by Peter Beaucage is free of charge for noncommercial use.
For other uses contact the author.
Please report any bugs, suggestions, comments to pab275@cornell.edu

Installation

Get and install:

Igor Pro (v. 6.2 or higher) – www.wavemetrics.net
Irena and Nika from Jan Ilavsky – usaxs.xray.aps.anl.gov or –link–

To install PeakTool:

You should have received two files: PF_MainProcedure.ipf and Boot PT.ipf

Installing Igor should have created a Wavemetrics folder in Documents, go there.

Copy "Boot PT.ipf" to the Igor Procedures folder.

Copy "PF_MainProcedure.ipf" to the User Procedures folder.

Basic instructions for use

I. Importing Data Into Igor

1. Launch Igor, in the Macros menu select first "Load Irena SAS Macros" and then "Load Peak Tools". You should now have a "SAS" menu and a "PB" menu in the menu bar.
2. Under SAS, select Data import & export > Import ASCII data. A large panel will pop up. General strategy is to proceed top to bottom.
3. Click select data path and choose the folder where your data are located (for data reduced using Wiesner group MATLAB macros, these are your *_int.txt files).
4. Type .txt into the small "Data extension box". Not necessary, but makes it easier to sort through files.
5. Check "skip lines" and select the appropriate number.
6. Click on one of your datasets in the "List of available files" box. Press "test" to the right.
7. Assign the columns. Normally column 1 = Qvec, 2 = Intensity.
8. Select appropriate Q units. Usually inv. Angstrom is correct.
9. If you want, you can use "trim data" or "reduce points" to clean up data… Likewise, if your file names are long, use "Truncate end"/"Truncate beginning"/"Remove Str from Name" to make them manageable.

10. Select (by shift-click or “Select all” button) the data you want to import in the box.
11. Push Import at bottom right.

II. Plotting data

Way more functionality than I want to summarize here, see Jan’s manual and videos for more help.

In short:

1. go to SAS > Plotting I. Panel will open.
2. Select “QRS” data format and choose a data set in the topmost drop down (Data fldr)
3. Click add data
4. Repeat as needed.

Note: you probably want to change the default options:

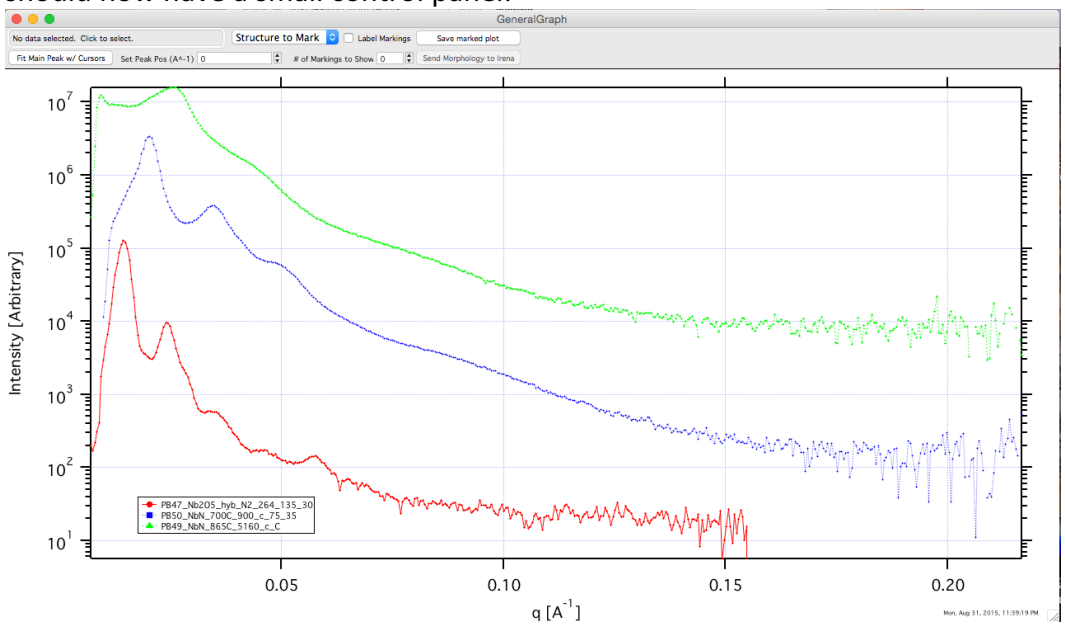
Turn off Log x axis

If plotting multiple datasets, set “Y offset” to sensible value so data are stacked.

Important known issue: changing a parameter in the Irena plot will reset PeakTool. So finalize how your data are displayed BEFORE you start tagging peaks!

III. Using Peak Tool

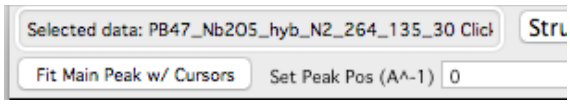
1. Under the “PB” menu, choose “Add Peak Tagging Tools to Plot”. Your plot should now have a small control panel:



2. To begin, click a data trace to select it. The textbox at the top left of the panel should update accordingly:

Before:

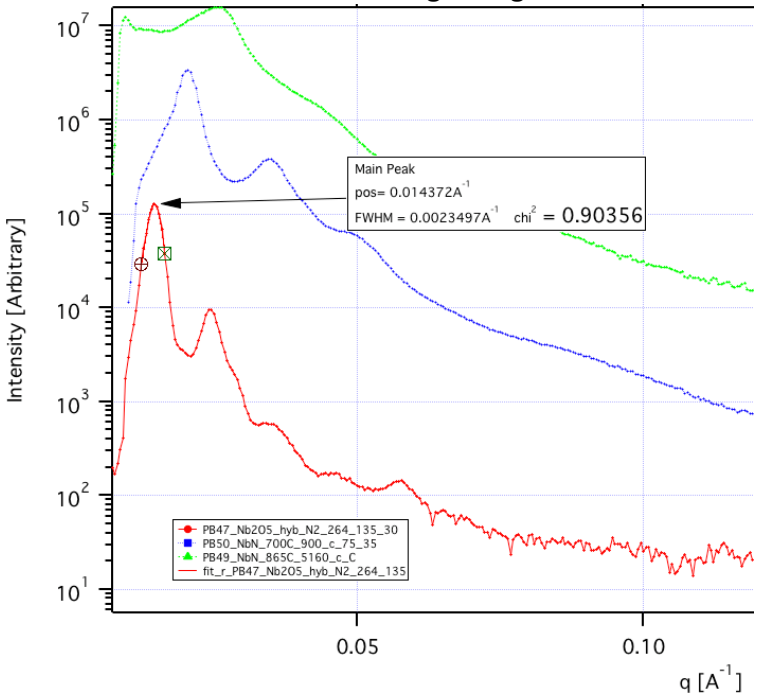
After:



3. At the bottom of your graph, you should have a small toolbar with two cursor areas: (if you don't see this, press ctrl/cmd-I to toggle)

Click and drag "A" to the left of your main peak, and "B" to the right of the peak. No need to be picky with the positions, these will be used as limits for fitting a Gaussian.

4. Click "Fit Main Peak w/ Cursors". Fitting routine will run, and resulting fit will be displayed on graph. Make sure it looks reasonable, then move on.
   If it doesn't look reasonable: Reduce the area to be fit until you get something appropriate. If all else fails, set the peak position manually using the textbox.
   If you get a warning about the chi-square value: this is the program saying that your fit isn't very good. If it looks OK, ignore it. If it looks funky but gets the right peak position, ignore it. If your fit looks bad, see previous.
5. Your curve should now have a tag. Drag it around to somewhere convenient.



6. To mark your peaks: From the "Structure to mark" dropdown, select an appropriate morphology.

The expected peak positions for this morphology will be tagged on your curve. You can adjust the number of markings shown and add labels using the controls at the top of the plot.
The tag will also be updated with the d(100) spacing and morphology.

If the tags don't fit, select another morphology from the dropdown.

7. To tag other data, just click on it and repeat from step 2.

To save your plot, use the button in the control panel (easy) or the File > Save Graphics dialog (harder, but allows you to choose size and file format).

You can double-click on traces to change their color and formatting.
You can manually edit the contents of textboxes/tags by double clicking.

IV. Bonus: Using Nika to reduce your data

< detailed instructions coming soon, check Jan's manual and videos for basic tutorial >