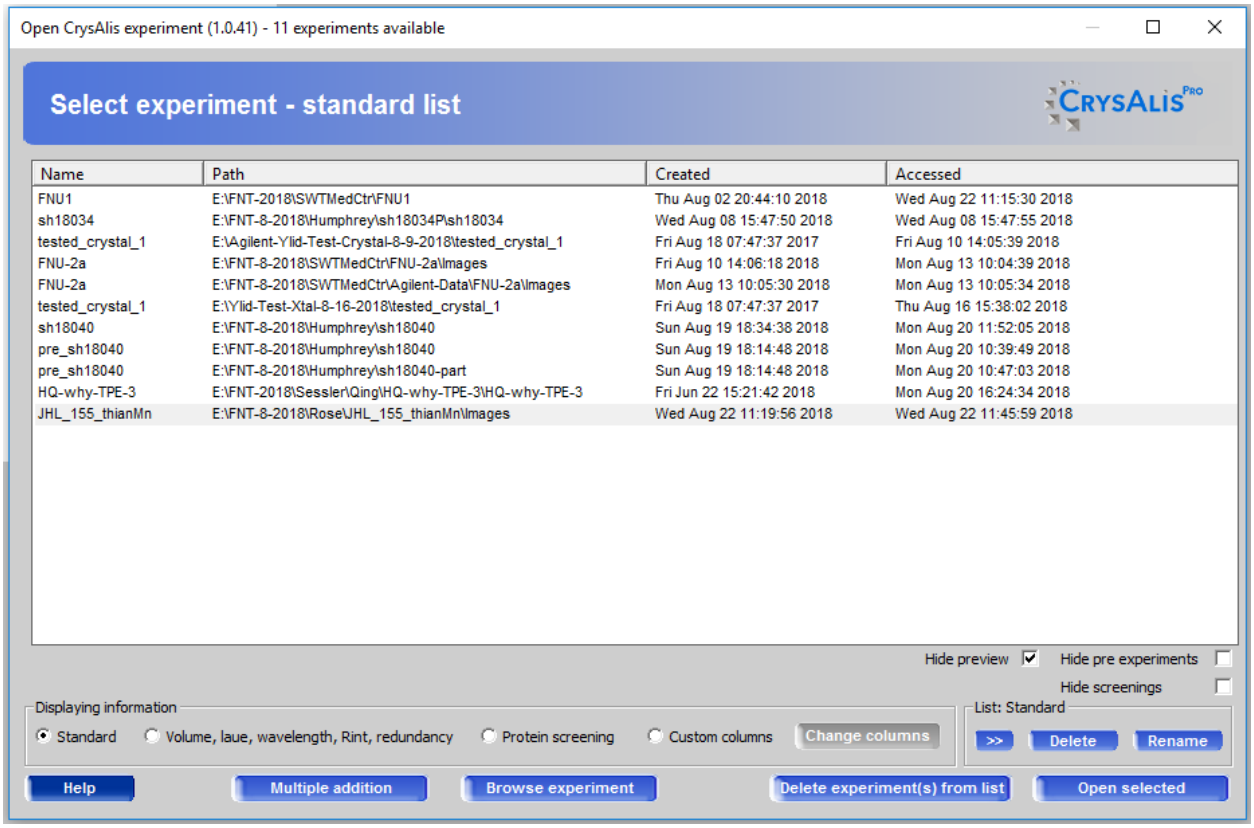
Using CrysAlisPro to process Saturn and Nonius Data sets

Open CrysAlisPro

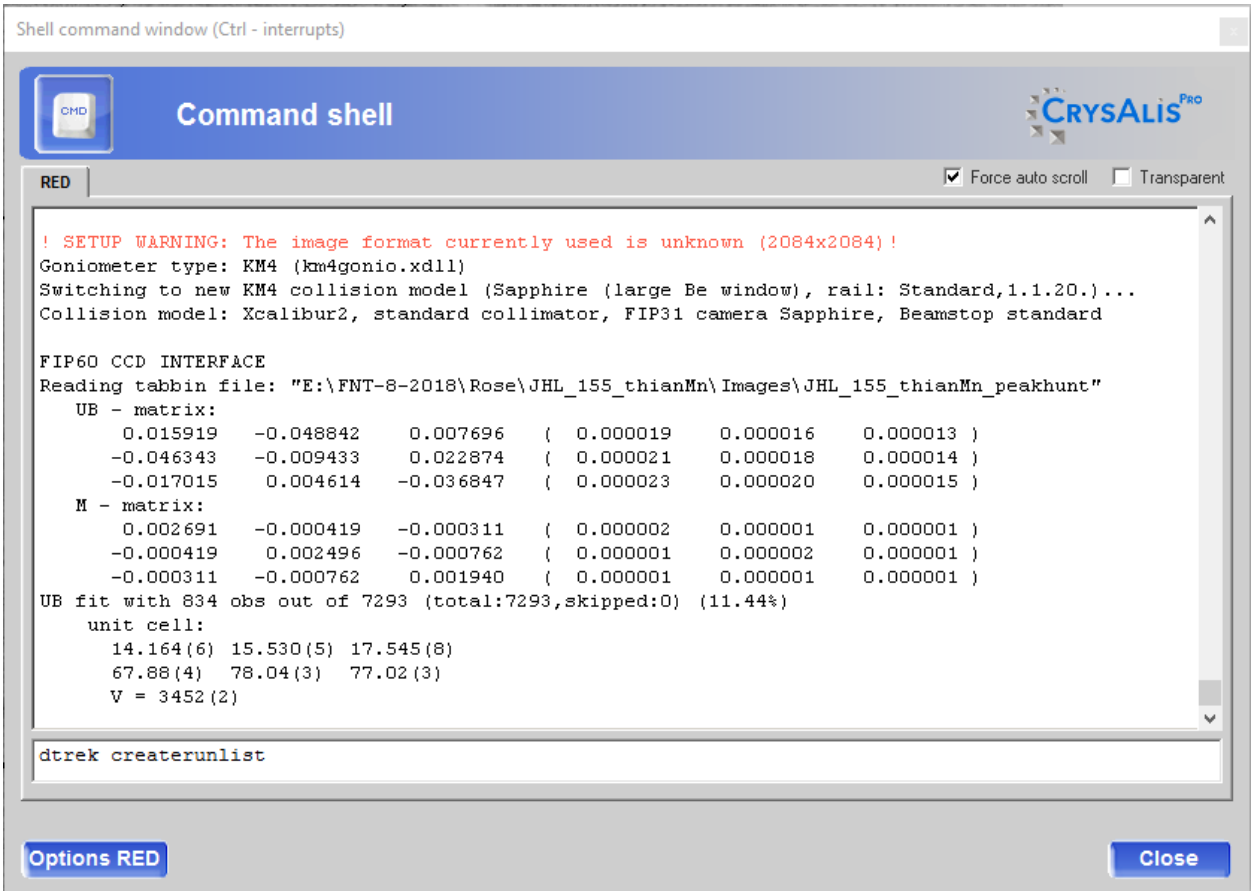


Select an experiment from the list. It doesn't matter which one you choose.

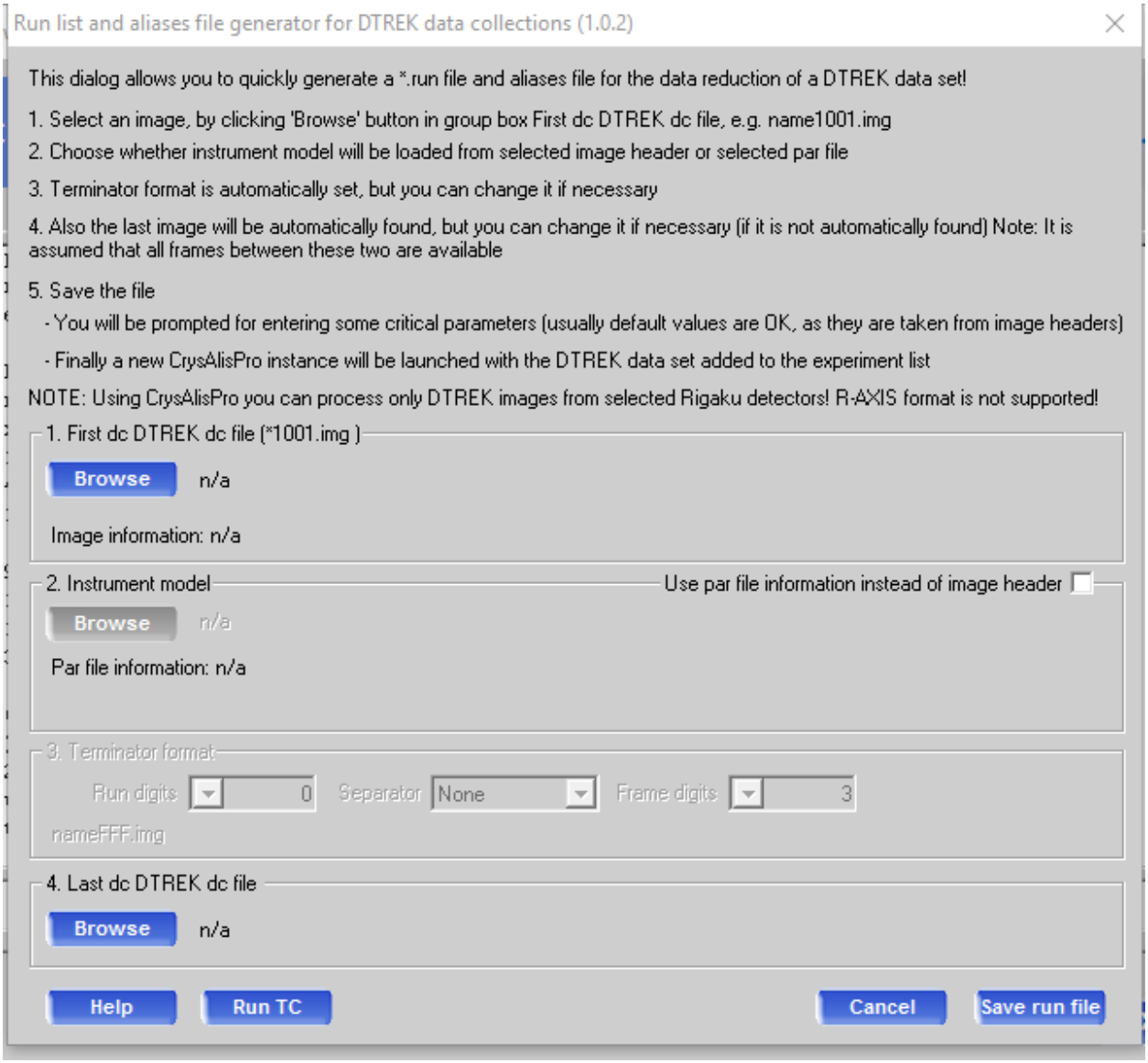
Select the command icon 

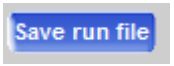
and type

Dtrek createrunlist for Saturn data or saxi createrunlist for Nonius data followed by enter

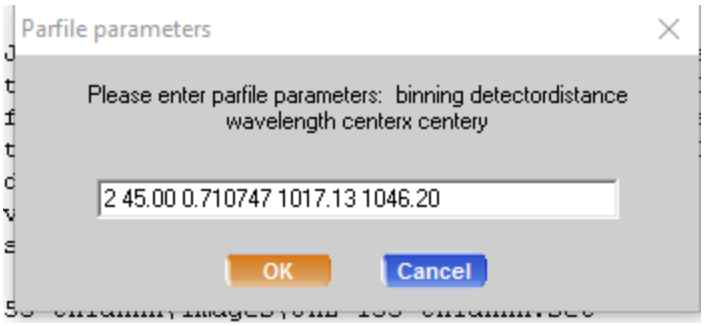


A menu will open where you select the data frames you want to use with the Browse button.



Select Browse for the first image in the first frameset and Browse to select the last image in the last frameset. Using Saturn data, you can ignore the initial screen data. For Nonius data, select the first frameset even if it is the initial screening data. You can deselect frames later. Select Save run file 

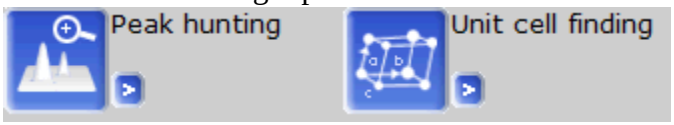
to read in the data. It may take a few seconds to read in all the data. When successful, a window will appear with the header information for the detector.



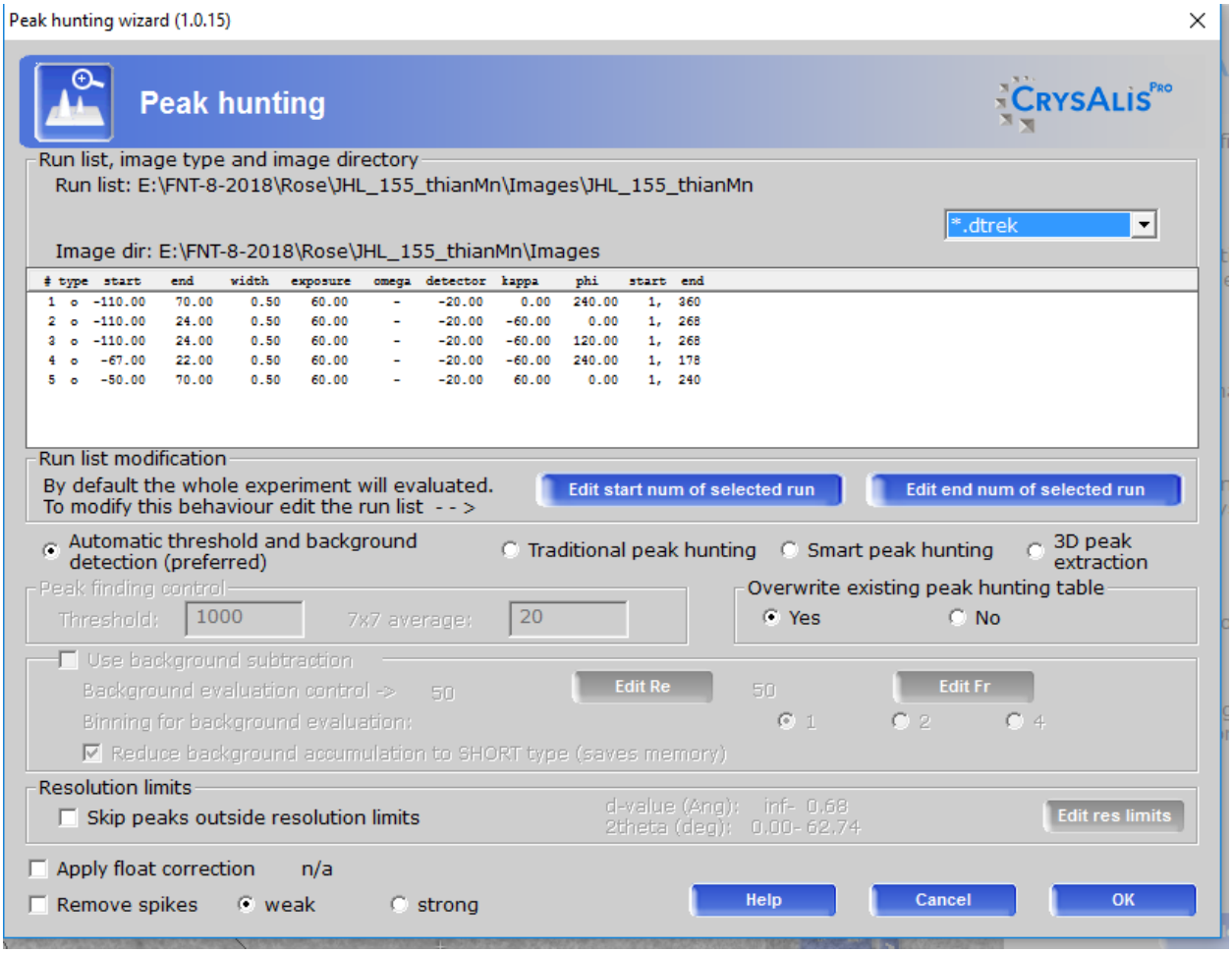
Select OK.

A new experiment will be created and highlighted for the Saturn/Nonius data set. Open the selected dataset.

A new CrysAlisPro menu will appear and will show the first image of the Saturn data. One thing you will notice immediately is that the Saturn frames are noisier than the Agilent frames. Some of this is due to the Atlas detector and some due to the lack of dezingering of the Saturn images (usually).

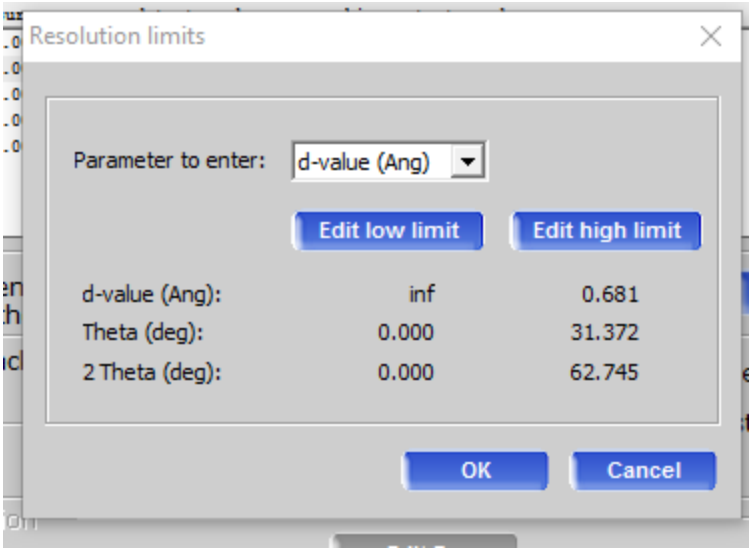
Basically, you proceed as you would for any Agilent data set. Select the Lattice Wizard  icon to begin peak selection and unit cell finding. Select Peak hunting 

followed by unit cell finding to get a starting unit cell. Left click the > symbol by the Peak hunting icon and select ‘Peak hunting with user settings’.



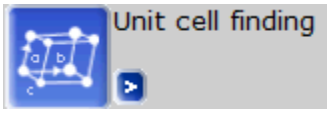
The frame data that was read in will be listed. I usually do two things at first. I will select one frameset and ignore the others when doing a peak search to save time. To bypass a frame set, select a frame set and then select 'Edit start num of selected run' and enter 0. Do this for all the frame sets you wish to bypass.

Secondly, I check the box 'Skip peaks outside resolution limits'. By default, CrysAlisPro will search the entire image which has resolution limits exceeding the useful range of the data scattering. Check the box and then select 'Edit res limits'.

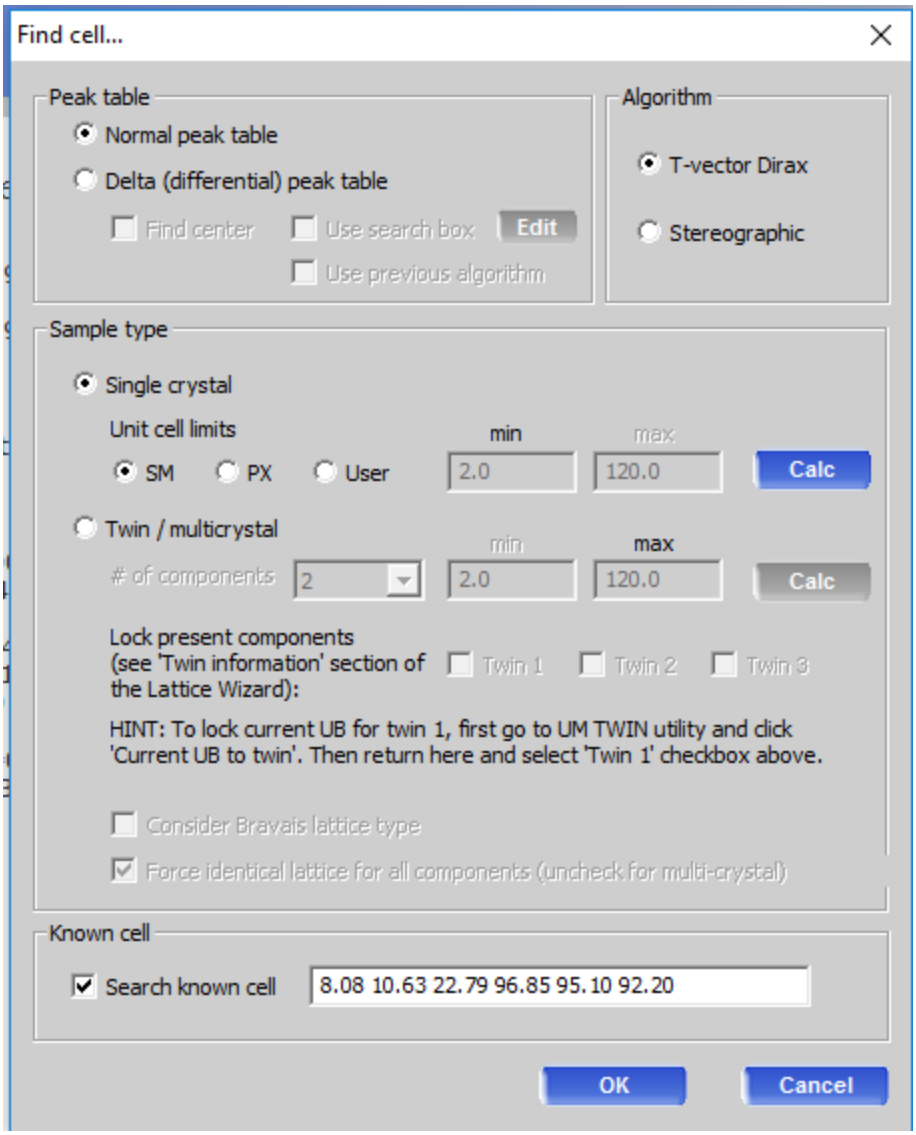


I usually select both low and high limits. For low limits, I enter 10 for the d-value. For the high limit, I will typically select 0.9 or something like that. These values will vary with the crystal and the data. This is only for the peak search and unit cell determination. For data integration, I use all the frames and use at least 0.83 or 0.77 for the high resolution limit. To use these values, select OK to get back to the Peak hunting menu.

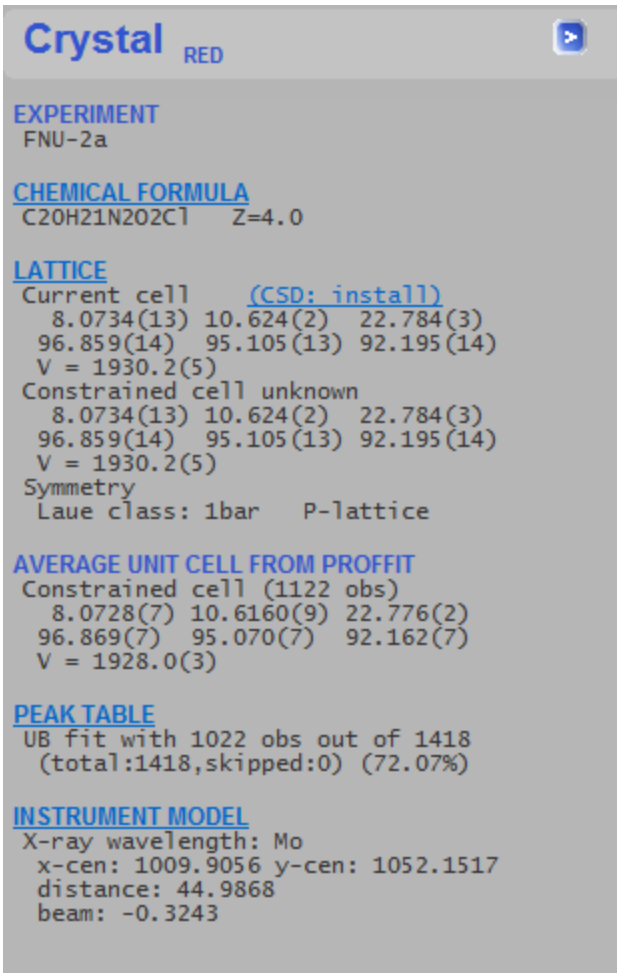
To begin the peak search, select OK in the Peak hunting menu. CrysAlisPro will go through the selected frames and generate a peak list just like CrystalClear. Because the frames are noisier, sometimes you have to work at getting a cell. If you have a good cell from CrystalClear and just want to take advantage of the superior data integration program in CrysAlisPro, you can enter the known cell in the 'Unit cell finding' menu. Left click the > symbol by the



icon, and select 'Unit cell finding with options'. At the bottom of the menu check the 'Known cell' box and enter the known unit cell.



And select OK. The Lattice wizard menu will appear with the unit cell. Look carefully at the results and check to see if the known cell is the current cell. Also, check the Peak Table and look at the percentage of reflections that match the cell. In this case, the value is 72%, which is good. If this number is much lower, sometimes the cell parameters need a little tweaking to come into agreement. Select Refine instrument model to refine the cell and instrument parameters to improve the fit. Sometimes an initial fit of 10% will improve to 30% and then 50% and higher with additional refinements. And sometimes not. Check the instrument model values listed on the right side of the CrysAlisPro menu. The easiest number to check is the crystal to detector distance.



For the Saturn, the default distance is 45.0, in the menu above it is 44.9868 mm. If the number is significantly different from the distance set for data collection, you will have to start over with the original values. The only way I know how to do this is to delete the file, filename_cracker.par, which contains the current information for the experiment and where filename is the name of the data set. Then copy filename.par to filename_cracker.par. These file will be located in the Image directory.

At this point, you have to reselect the experiment  and start over.


Lattice wizard (1.0.35)
Lattice wizard
CRYSALIS PRO
LATTICE
Current cell (CSD: install)
8.0763(13) 10.627(2) 22.792(3) 96.854(14) 95.100(13) 92.196(14) 1932.1(5)
Lattice reduction
selected cell
8.0763 10.6271 22.7920 96.8539 95.0998 92.1956 aP 44
reduced cell
8.0763 10.6271 22.7920 96.8539 95.0998 92.1956 1932.1
PEAK TABLE
Peak hunting table
UB fit with 1022 obs out of 1418 (total:1418,skipped:0) (72.07%)
INSTRUMENT MODEL
Goniometer
beam: -0.31826 alpha: 50.00000 beta: 0.00000
om zero: 0.00877 th zero: -0.04382 ka zero: 0.00000
Detector
x-rot: -0.04081 y-rot: 0.01944
x-cen: 1009.87941 y-cen: 1052.12532 distance: 45.00772
Wavelength Mo (Ang): A1 0.70930 A2 0.71359 B1 0.63229
Refinement
res: 0.010487, da=0.008042, sx=0.000879, sy=0.001493
h=0.004302, k=0.003651, l=0.003235
#ref: 1018 (skipped: 2)
Peak hunting
Unit cell finding
Ewald explorer - reciprocal space
Reindexation with current cell
Refine instrument model
Lattice transformation
Twinning - multi-crystals
Incommensurates / Quasi-crystals
LOAD
Load information
SAVE
Save information
Ewald3D
Unwarping - Precession images
Log window
Close