

Brute Force Data Integration in CrysAlisPro

For some problem data sets, you can use a feature in CrysAlisPro using a batch job to adjust several parameters sequentially when integrating your data. This allows you to adjust parameters such as mask size, background measurement, resolutions limits, etc. Essentially, it allows you to do data reduction with options and change many parameters. For the different changes you make, CrysAlisPro will generate an hkl and cif_od file for each set of changes. You can then take all the different hkl files and copy them into the same OLEX2 or WinGX folder and run least-squares using the different hkl files and choose the one that gives the best result in terms of R1, wR2, Rint, etc.

This procedure is discussed in a video describing data processing of Electron Diffraction data. I have uploaded the video to my UTBox account in the folder, 3DED-workshop-videos. This procedure is described in the video CrysAlisPro data reduction. It is discussed near the end of the video.

Use care when using one hkl file over another. The value for wR2 is influenced by the weighting scheme used so you should allow the weighting factors to refine. This is the default in OLEX2 but the weight can be fixed. I look at the $I/\sigma(I)$ values, the % completeness and the GooF value as well as the agreement factors.

Don't expect dramatic differences but you may lower certain parameters so that they become acceptable to the CIF police.

Open your data in CrysAlisPro.

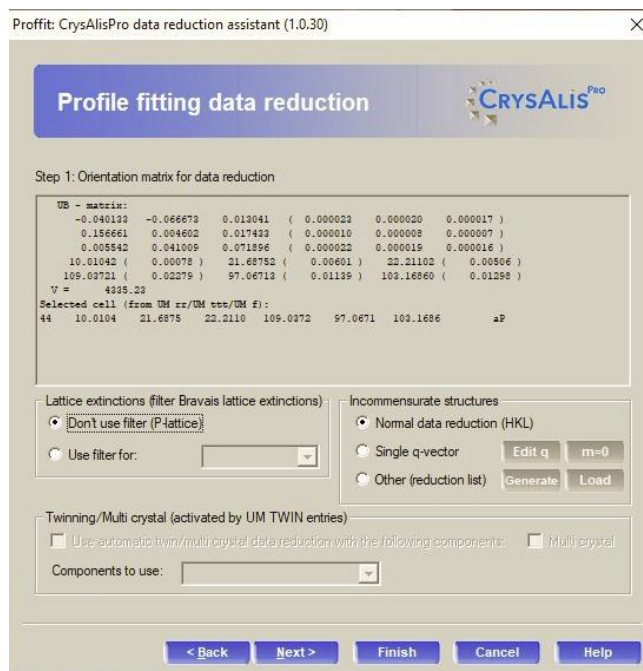


Select the Command Shell

Type xx profitloop (note the two f's) and hit the enter key



The data reduction menu will appear. Here you can remove frames that are unusable because of ice buildup or extremely high background because the X-ray beam clips the steel pin of the cryoloop.



Bad backgrounds usually occur at the end of the framesets. You can use the ‘Edit end num of selected run’ to instruct CrysAlisPro to skip the affected frames starting at the frame number you select. If the issue is frames from the start of a run use ‘Edit start num of selected run’.

Proffit: CrysAlisPro data reduction assistant (1.0.30) ×

Profile fitting data reduction

Step 2: Experiment run list for data reduction

Run list: E:\FNT-2022\Rose\Brenna\bc855_GREEN\bc855_GREEN

*.rodhypix ▾

Image dir: E:\FNT-2022\Rose\Brenna\bc855_GREEN\frames

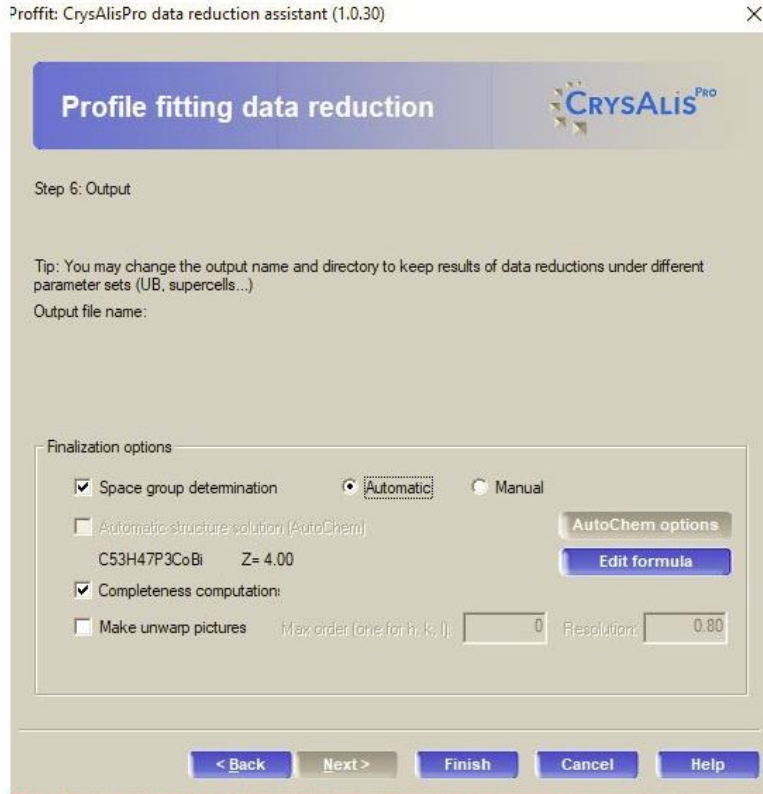
#	type	start	end	width	exposure	omega	detector	kappa	phi	start	end
1	o	-11.00	16.00	0.50	17.00	-	-47.29	23.00	-46.00	1,	54
2	o	-173.00	-95.00	0.50	62.00	-	-104.52	-23.00	148.00	1,	156
3	o	-122.00	-37.00	0.50	17.00	-	-47.29	-23.00	148.00	1,	170
4	o	-59.00	-32.00	0.50	62.00	-	-104.52	77.00	-150.00	1,	54
5	o	40.00	116.00	0.50	17.00	-	47.29	23.00	-46.00	1,	152
6	o	-110.00	-35.00	0.50	62.00	-	-104.52	125.00	0.00	1,	150
7	o	-13.00	23.00	0.50	17.00	-	47.29	-23.00	148.00	1,	72
8	o	95.00	178.00	0.50	62.00	-	104.52	23.00	-46.00	1,	166
9	o	-90.00	-22.00	0.50	17.00	-	-47.29	125.00	90.00	1,	136
10	o	-66.00	25.00	0.50	17.00	-	-47.29	77.00	-60.00	1,	182
11	o	-25.00	13.00	0.50	17.00	-	47.29	-19.00	0.00	1,	76
12	o	-21.00	17.00	0.50	17.00	-	47.29	-19.00	-60.00	1,	76

By default the whole experiment will be evaluated. To modify this behaviour edit the run list -->

Edit start num of selected run
Edit end num of selected run

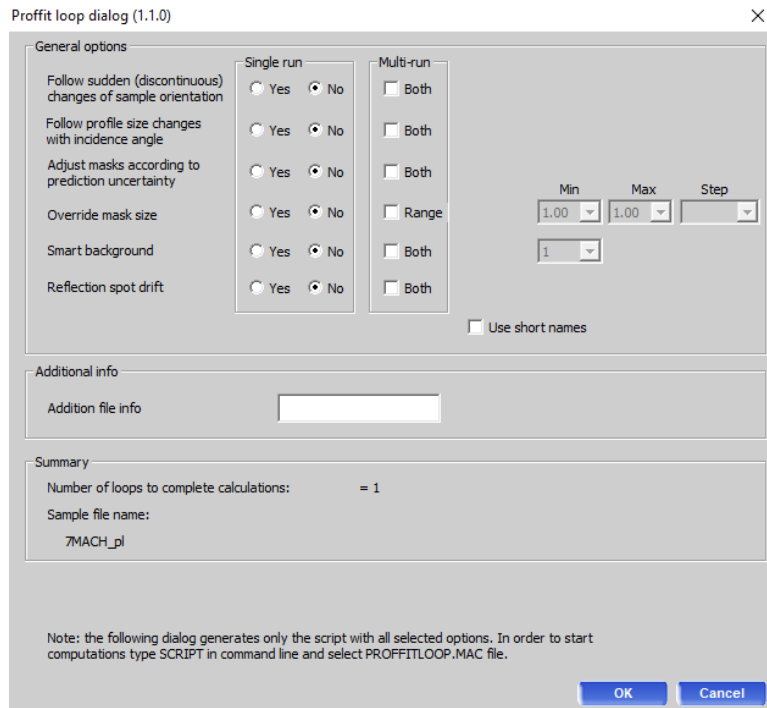
< Back
Next >
Finish
Cancel
Help

Keep selecting [Next](#) until you come to the output menu.



Be sure to select **Automatic** if you want the data reduction to continue in background mode. If you select manual, you will need to intervene at the end of each integration cycle. There may be many cycles depending on your choices.

Select **Finish**. The profile fitting loop selections menu will appear. I use the 'Use short names' feature because it is easier to see the full name of the hkl file used in the refinement. There should be some slight differences in the refinement values depending on the selections chosen. With some luck, you can turn a marginal refinement model into one that is satisfactory to a reviewer.



As you select different options, the value for the number of loops to complete calculations will change. As you will see, this number can be large. With each selection, the sample file name will appear indicating the name of the hkl and cif_od files created.

When you have completed your selections, hit OK. The Command Shell will appear. Type **script** in the shell. The data directory will come up and a file 'proffitloop.mac' will appear. Double click on this file to start the data reduction process. The integration will run sequentially. You can follow the progress in the Start/Stop window under Data Reduction.

