Phenix and CCP4
Data input

Phenix

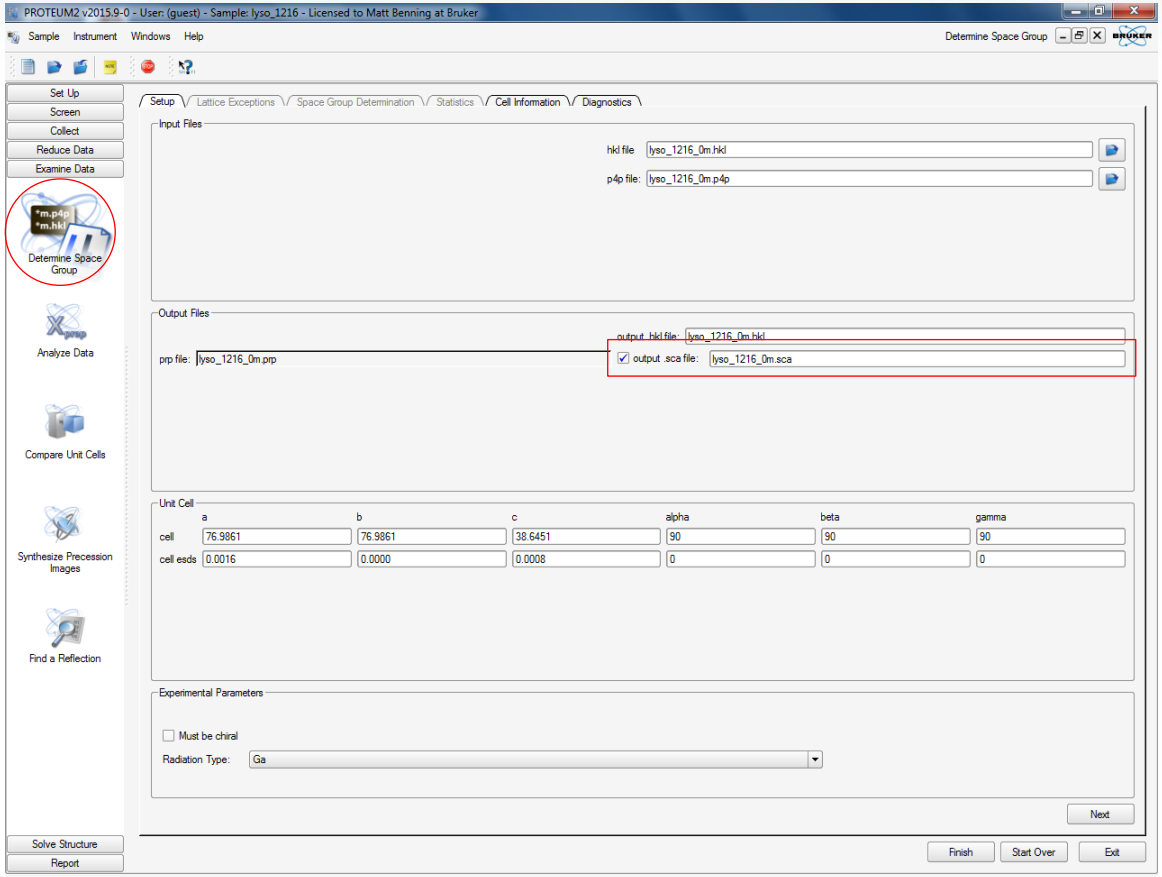
- Reads both SHELX HKLF4 (intensity, F^2), Scalepack and mtz files.

CCP4

- Use Import merged data to read in a Scalepack file.
- Use Convert to/modify/extend (f2mtz) MTZ to read in a SHELX HKLF4 file. However will the resulting mtz file will be merged.
- Use pointless to create an unmerged mtz file which can be imported into Aimless.
- Use f2mtz to inport a SHELX phs file from phasing runs.

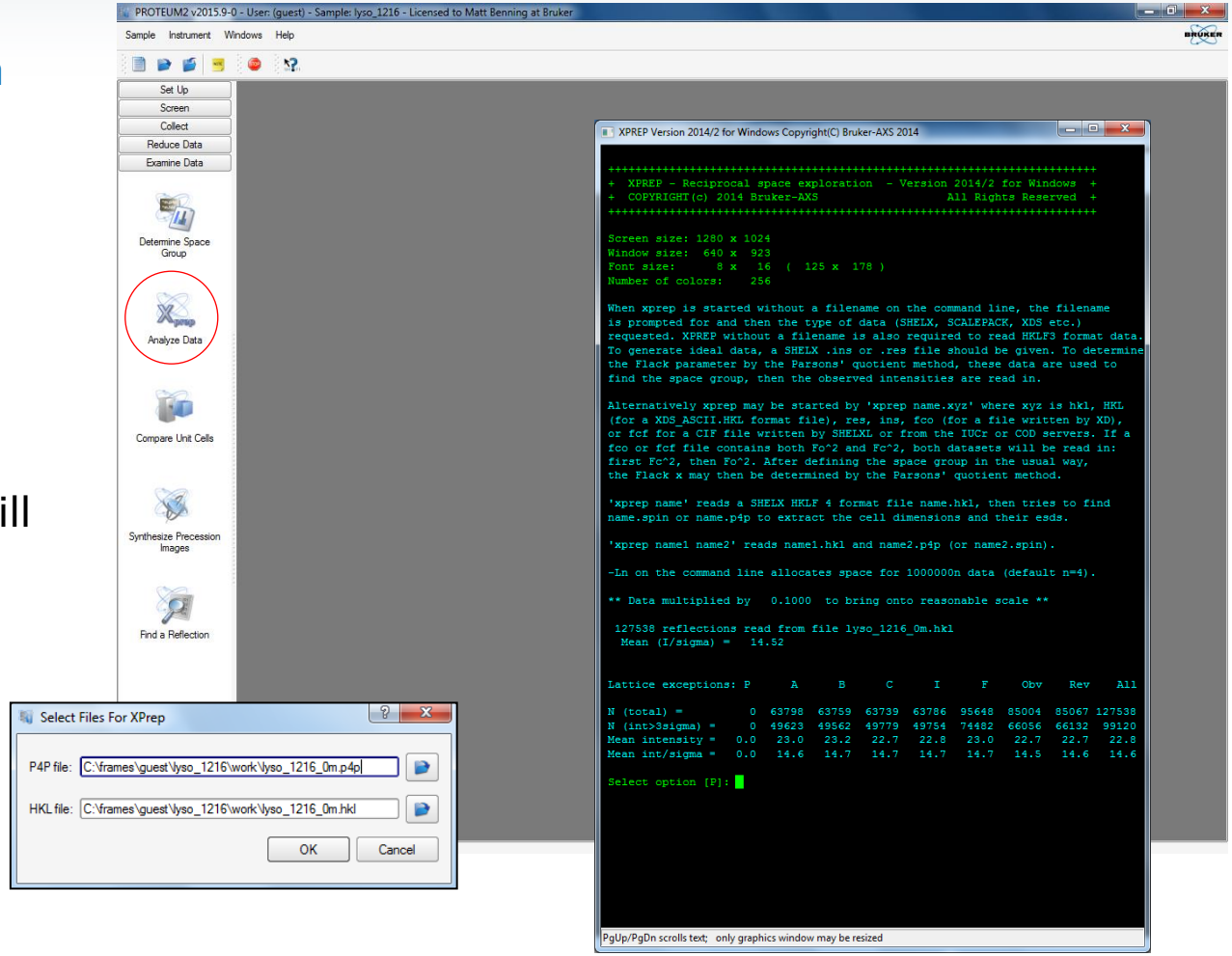
Determine Space Group
Writing out Scalepack File

- Click Determine space group
- Click the output sca file button and run it as you normally work
- The sca file will be written to the work directory when you finish



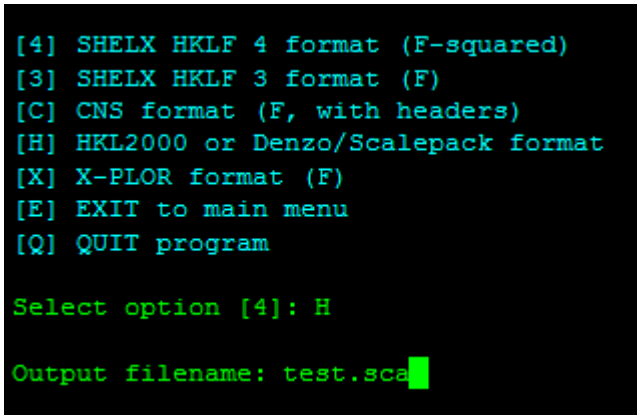
XPREP
Writing out Scalepack File

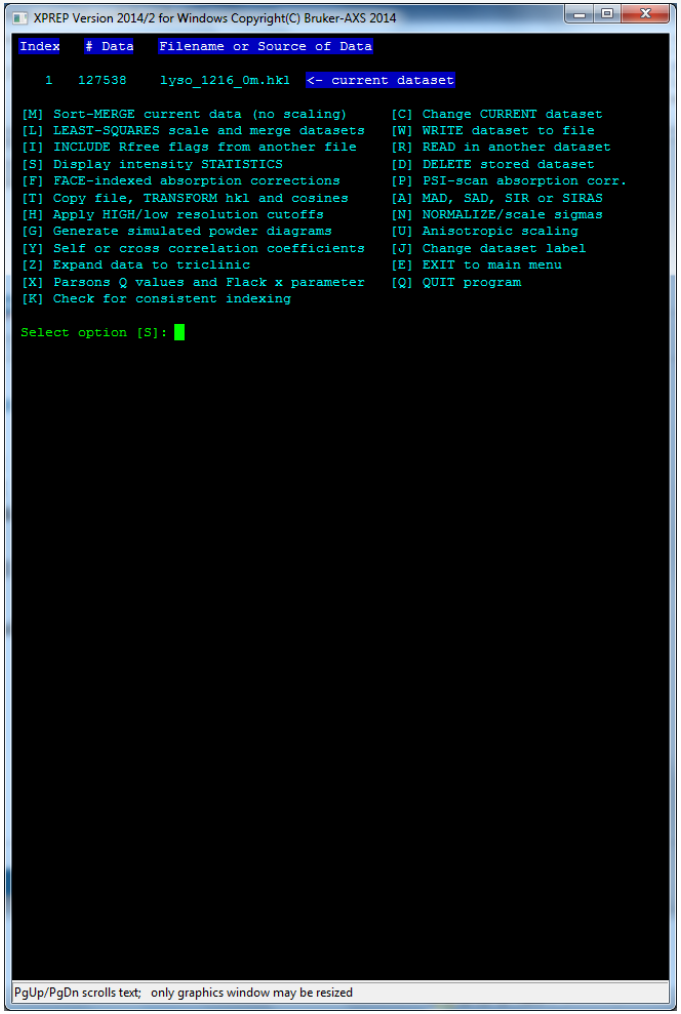
- Select Analyze Data from the Examine Data menu
- Browse for the correct p4p and HKL file if not already shown the files box and click Ok
- The XPREP window will open
- Hit the CR once, this will take you to the main menu



XPREP
Writing out Scalepack File

- Follow the normal path to select the metric symmetry and space group
- At the main menu, select option D for Read, Modify and merge datasets
- Select option W to write out a HKL file
- Select option H for exporting a Denzo/scalepack formatted file and input a filename





Inputting data to Phenix
SHELX or Scalepack HKL file

Phenix will read either a SHELX or Scalepack formatted file. However with the SHELX format, you have to define whether it is a HKLF4 (intensities) or HKLF3 (amplitudes). Typically you will be reading in intensities.

- If the name of the file is data.hkl, make a copy of the file in the same directory and call it data.hkl=hklf4
- Load the data.hkl=hklf4 into Xtriage
- Input the cell constants and space group
- Outputs a mtz file

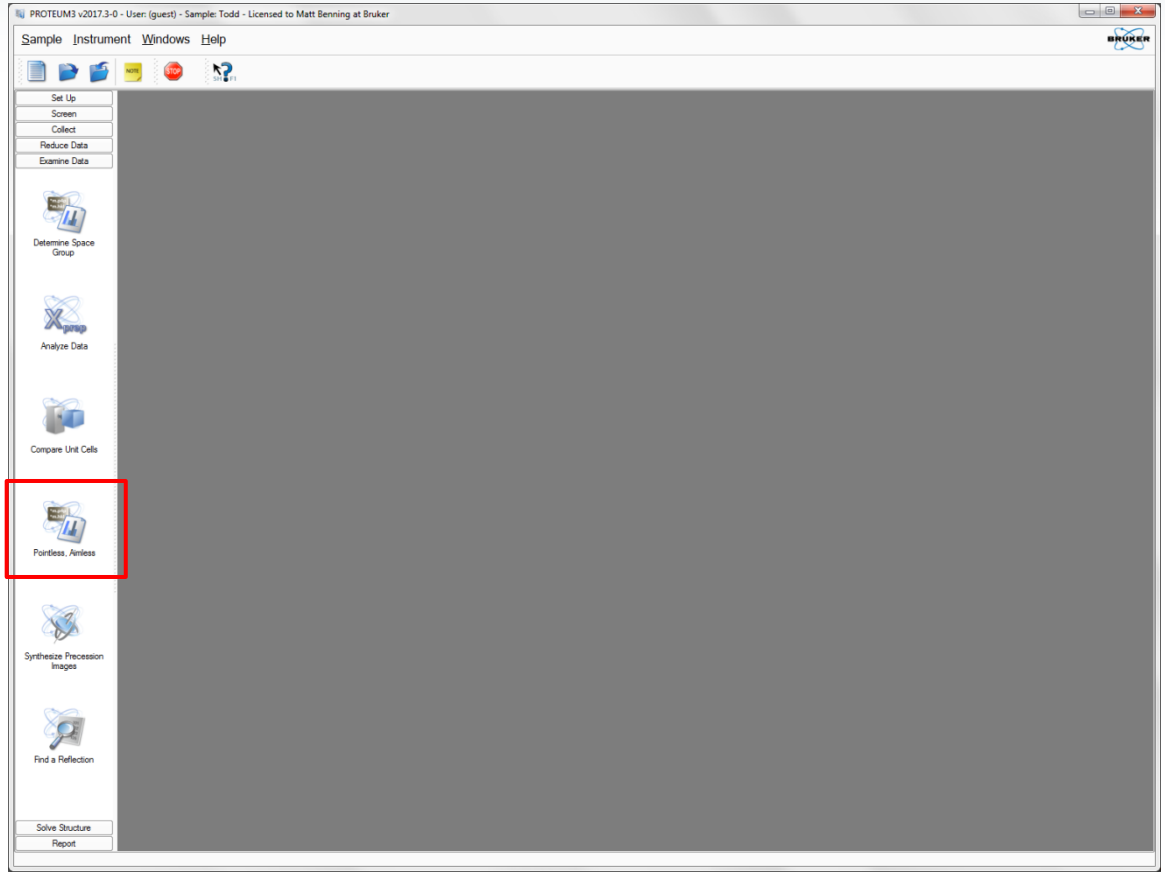
Pointless, Aimless

If you have CCP4 installed, add the following 3 lines to the end of the bn-config.py file

- ccp4 = "C:/CCP4-7/7.0"
- ccp4_range = [22.0,1.85]
- ccp4_autoprocess = True

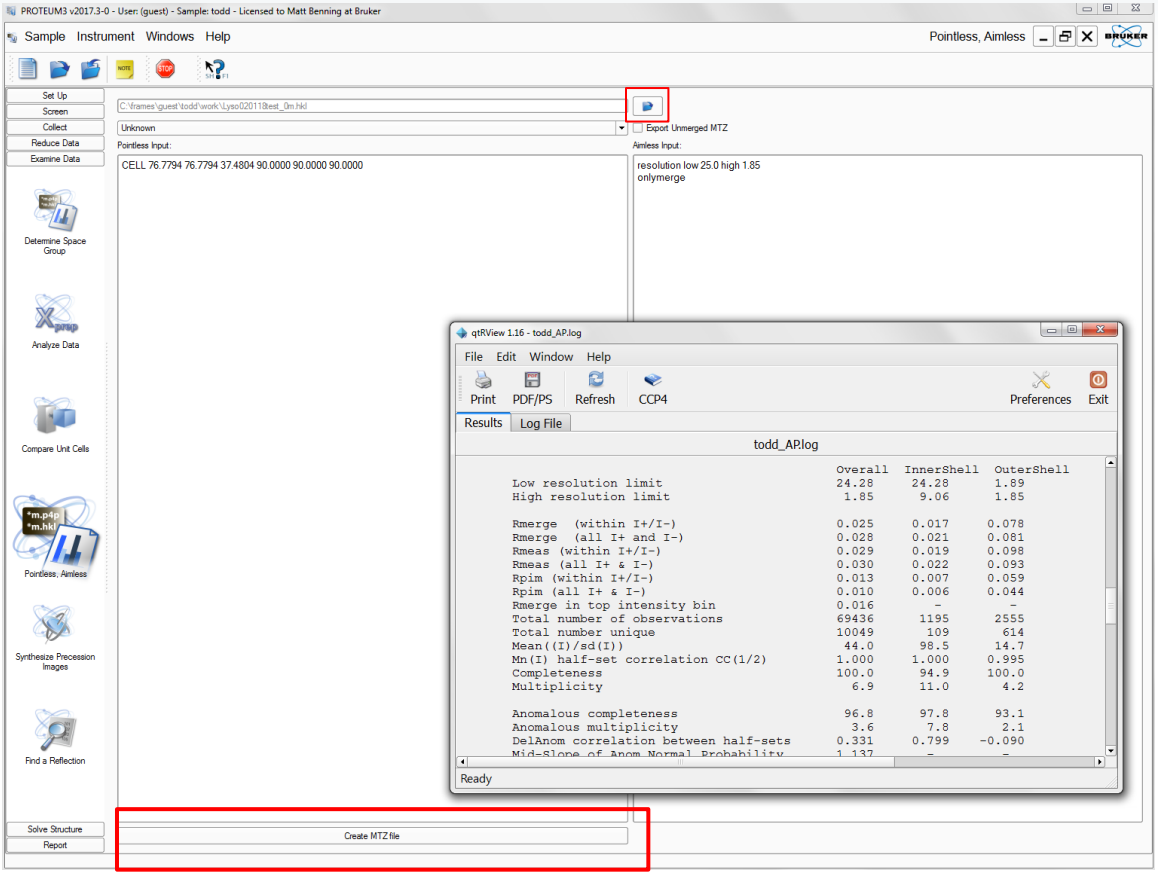
Pointless, Aimless

- Open the “Examine Data” menu
- Select the “Pointless, Aimless” icon



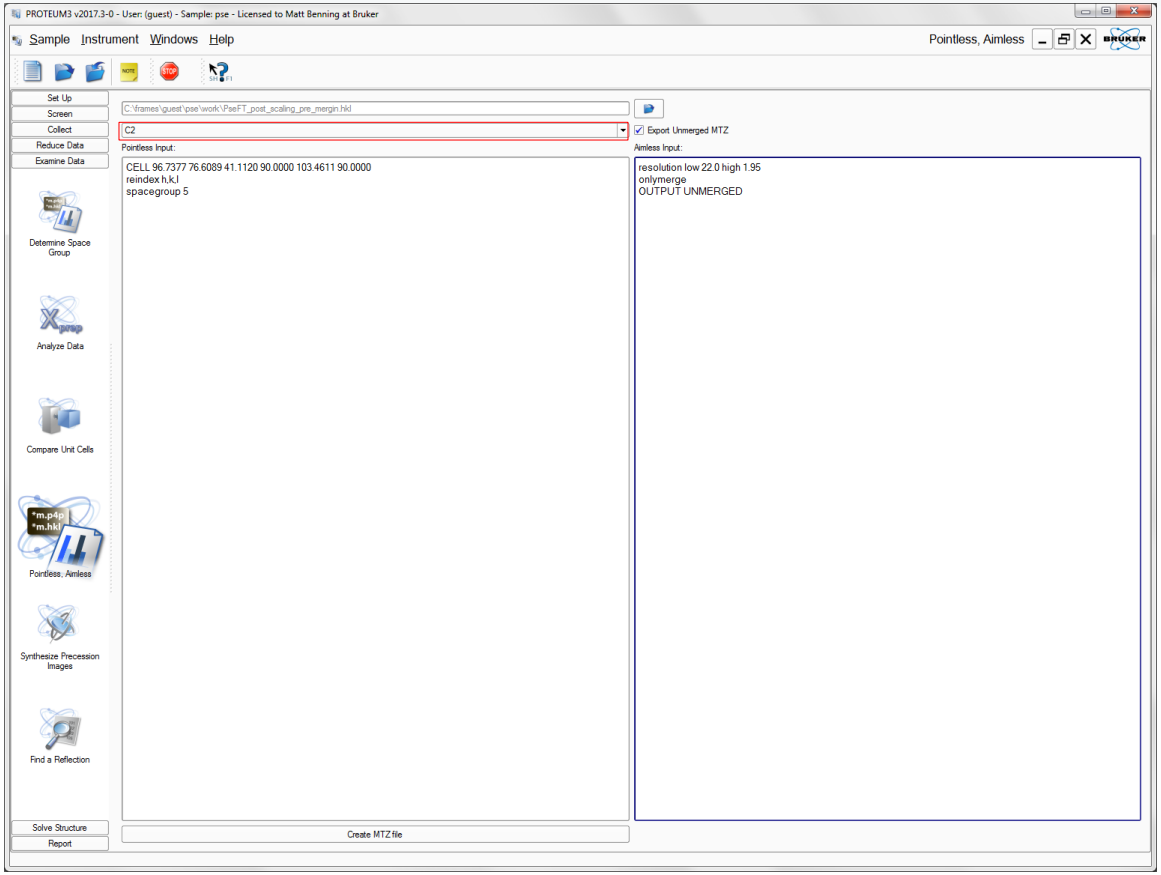
Pointless, Aimless

- If there is no MTZ file in the work folder, PROTEUM will automatically run Pointless and Aimless based on default values and display the aimless output.
- Default resolution 25 – 1.85 Å
- The pointless and aimless fields are editable so you can add keywords, change the defaults and click "create MTZ file" at the bottom left to rerun the programs. The new Aimless log will appear when both programs are finished.
- If the space group is not assigned (default), PROTEUM lets pointless perform a space group search.
- The plugin will search for the *HKL filename*_0m.hkl in the work directory but you can also search for a HKL file using the browser button.

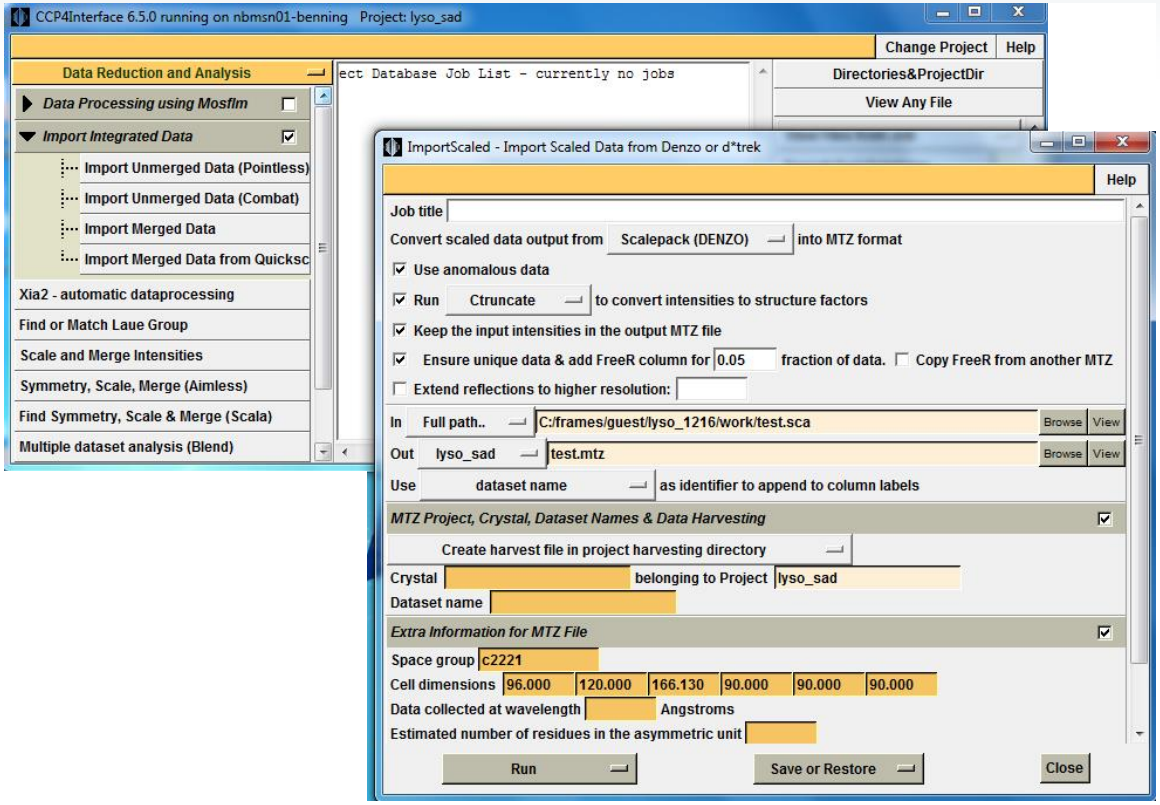


Pointless, Aimless

- If you want to assign a space group, select the desired group in the box below the input HKL filename. This will fix the space group to the that group assigned.
- A merged MTZ file is written out by Aimless, if you want to write out a unmerged MTZ file as well, check the "Export Unmerged MTZ"
- Output files are written to the work folder.
  - *Entry prefix*_AP.log is the output logfile from Aimless
  - *HKL filename*_merged.mtz is the merged MTZ file output by Aimless
  - *HKL filename*_umerged.mtz is the corresponding unmerged MTZ

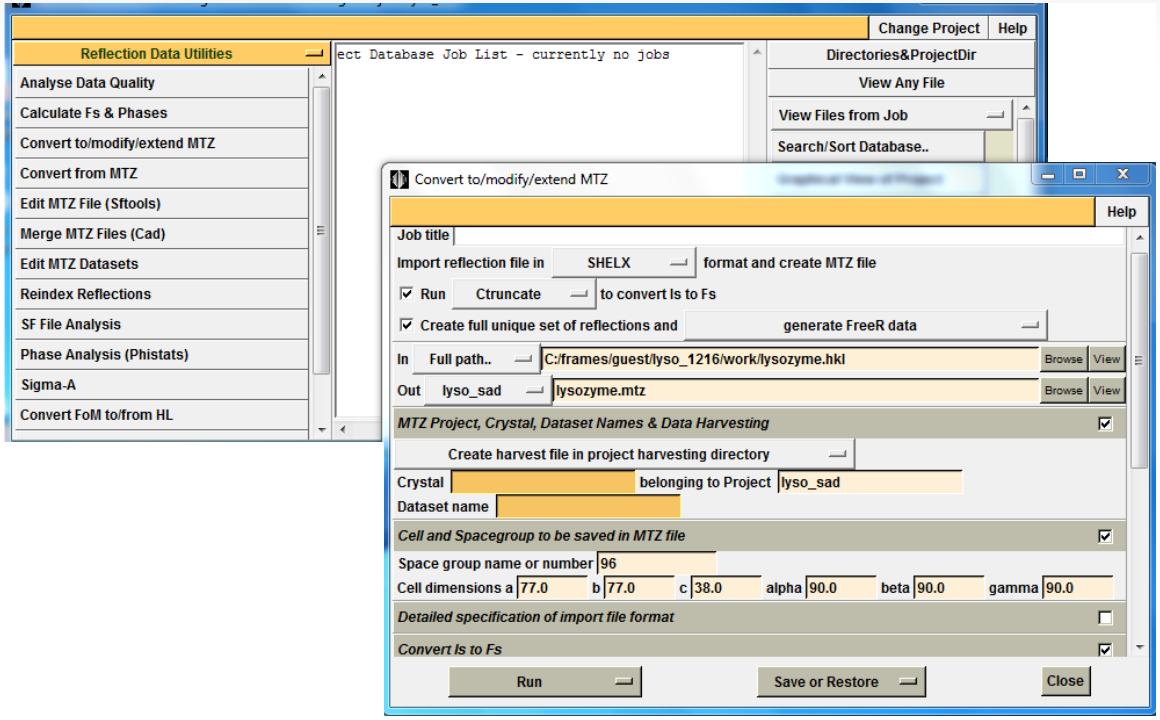


Inputting data to CCP4
Scalepack file



- From the Data Reduction and Analysis menu, select Import integrated Data>Import Merged Data
- Browse for the scalepack file
- Fill in any missing information

Inputting data to CCP4
SHELX HKLF4 file



- From the Reflection data Utilities, select Convert to/modify/extend MTZ
- In the input window, change the Import reflection filetype to SHELX
- Browse for the SHELX HKL file
- Input the Space group and Cell information and any other missing information

Using Pointless to Create MTZ
File prep

- With a HKL file written by SADABS, you have to remove the lines at the end of the file after the last reflection line (highlighted in blue below). If you write out a HKLF4 file from XPREP, you can skip this step.

```
 9   1 -23 2.02095 11.0166   1
  0   0   0    0.00    0.00   0

 _exptl_absorpt_process_details
;
 SADABS 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D.,
 J. Appl. Cryst. 48 (2015) 3-10
;
 _exptl_absorpt_correction_type    multi-scan
 _exptl_absorpt_correction_T_max  1.0000
 _exptl_absorpt_correction_T_min  0.8067
 _exptl_special_details
;
 The following wavelength and cell were deduced by SADABS from the
 direction cosines etc. They are given here for emergency use only:
 CELL 1.54369   42.505   45.457   47.886  101.541  114.565   89.042
;
```

Using Pointless to Create MTZ

Pointless –c hklin *filename*.hkl hklout *filename*.mtz <pointless.inp

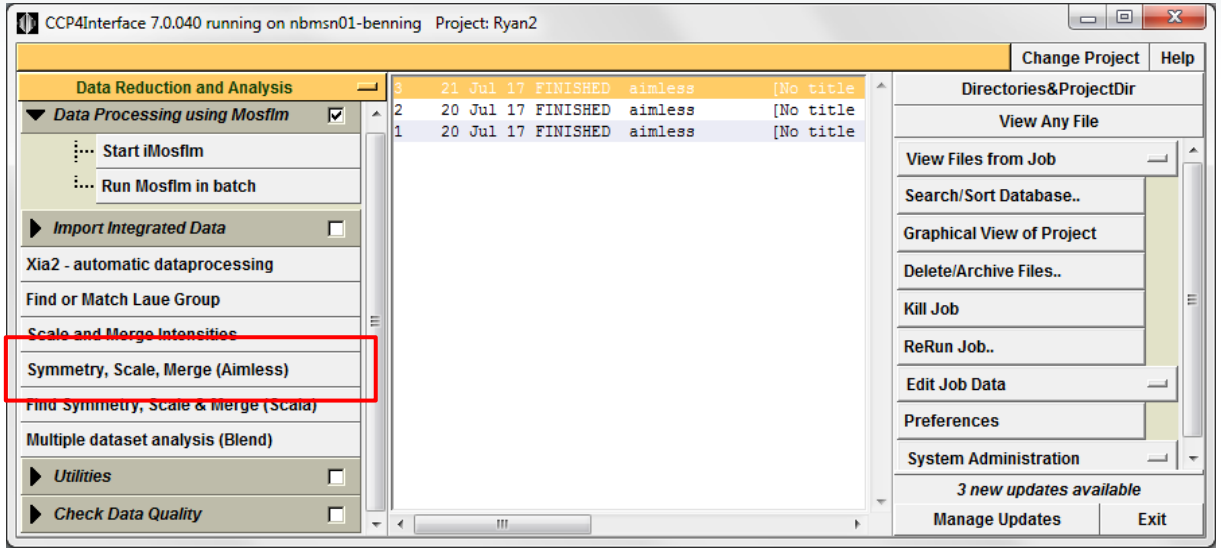
To create the input file you only need to add the three lines below. Just update the cell and space group information (space group is optional). The cell constants just have to be separated by a space.

- Pointless.inp

  cell 119.3466 45.1348 74.2698 90.0000 120.9434 90.0000
  reindex h,k,l
  spacegroup 19

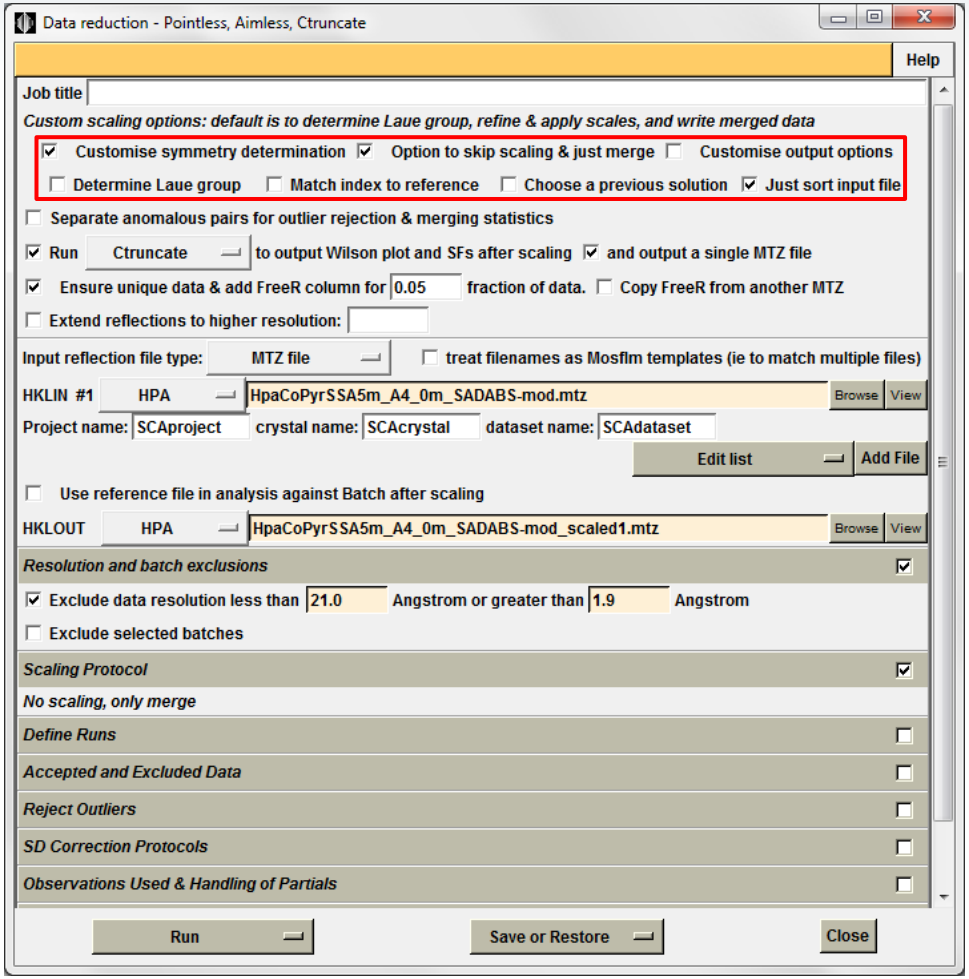
Importing SHELX mtz file into Aimless

- Click on “Symmetry, Scale & Merge” as you normally would to run Aimless



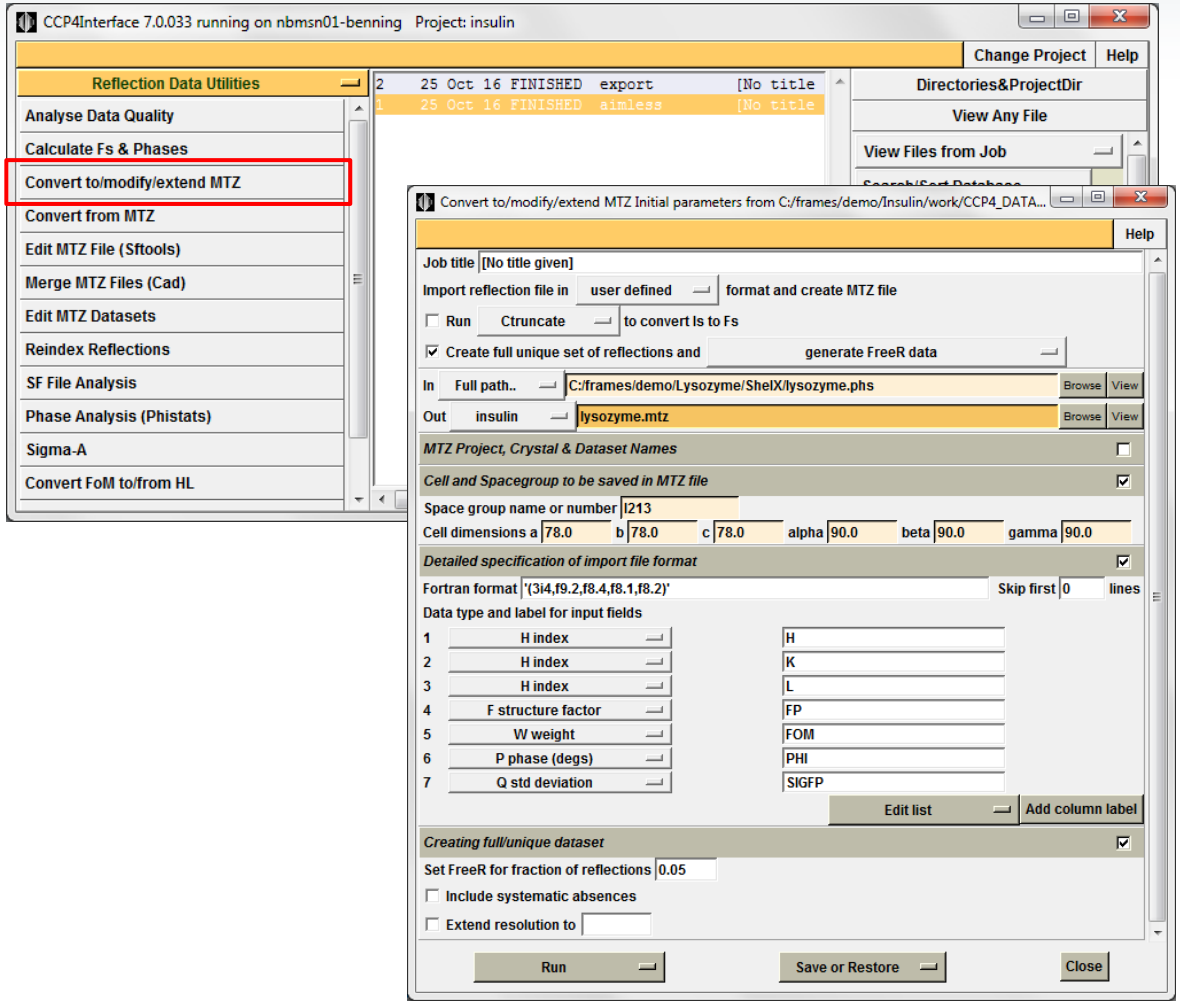
Running Aimless

- Select "Option to skip scaling & just merge"
- To disable Aimless from changing the space group click "Customise symmetry determination" and uncheck "Determine Laue group"
- Click to add a Rfree flag
- Browse for the mtz file created with pointless
- Set the resolution range if desired



Converting a PHS file to MTZ format

- Click on "convert to/modify/extend MTZ" under the Reflections data Utilities menu
- Set import file to "user defined"
- Click the box to generate a FreeR data
- Browse for the phs file and assign a output mtz filename
- Input the space group and cell dimensions
- Input the file format
  - 3i4,f9.2,f8.4,f8.1,f8.2
- Set the data type and labels as shown
- Click run



Converting a PHS file to MTZ format

f2mtz –c hklin *filename*.hkl hklout *filename*.mtz <phs_to_mtz.inp

To create the input file you only need to add the three lines below. Just update the cell and space group information (space group is optional). The cell constants just have to be separated by a space.

- Phs_to_mtz.inp

  symmetry H3
  cell 78.0 78.0 78.0 90.0 90.0 90.0
  format '(3i4,f9.2,f8.4,f8.1,f8.2)'
  skipline 0
  labout H K L FP FOM PHI SIGFP
  ctypout H H H F W P Q
  PNAME S100
  DNAME
  XNAME