CrysAlis^{Pro}: Data reduction different image formats

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X-ray Group Software Manager

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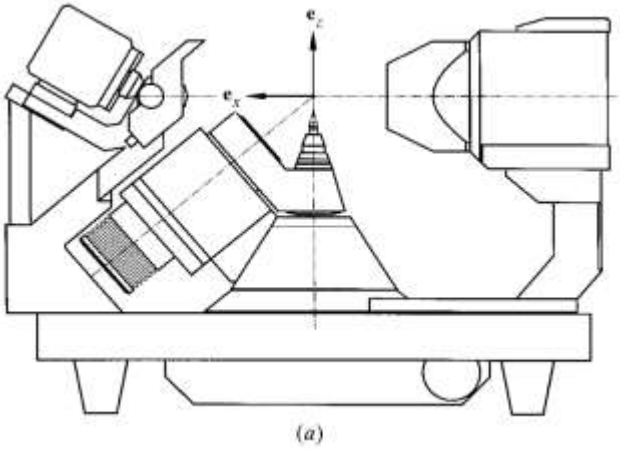
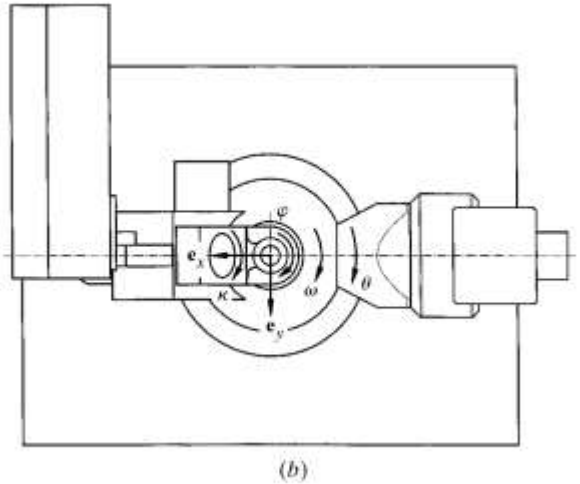
Area detector diffraction experiments

- Understand the experiment
- Goniometer description
- Sense of rotation
- Area detector ‘perspective’
- Zero points

- Kappa vs. Euler geometry





W. A. Paciorek, M. Meyer and G. Chapuis: 'On the geometry of a modern imaging diffractometer'; *Acta Cryst.* (1999). **A55**, 543-557

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Workflow on in-house instruments

- Describe instrument
- Run fully automatic calibration experiment describing fully the instrument at any distance
- Run test data collection on standard sample
- Run new experiment.

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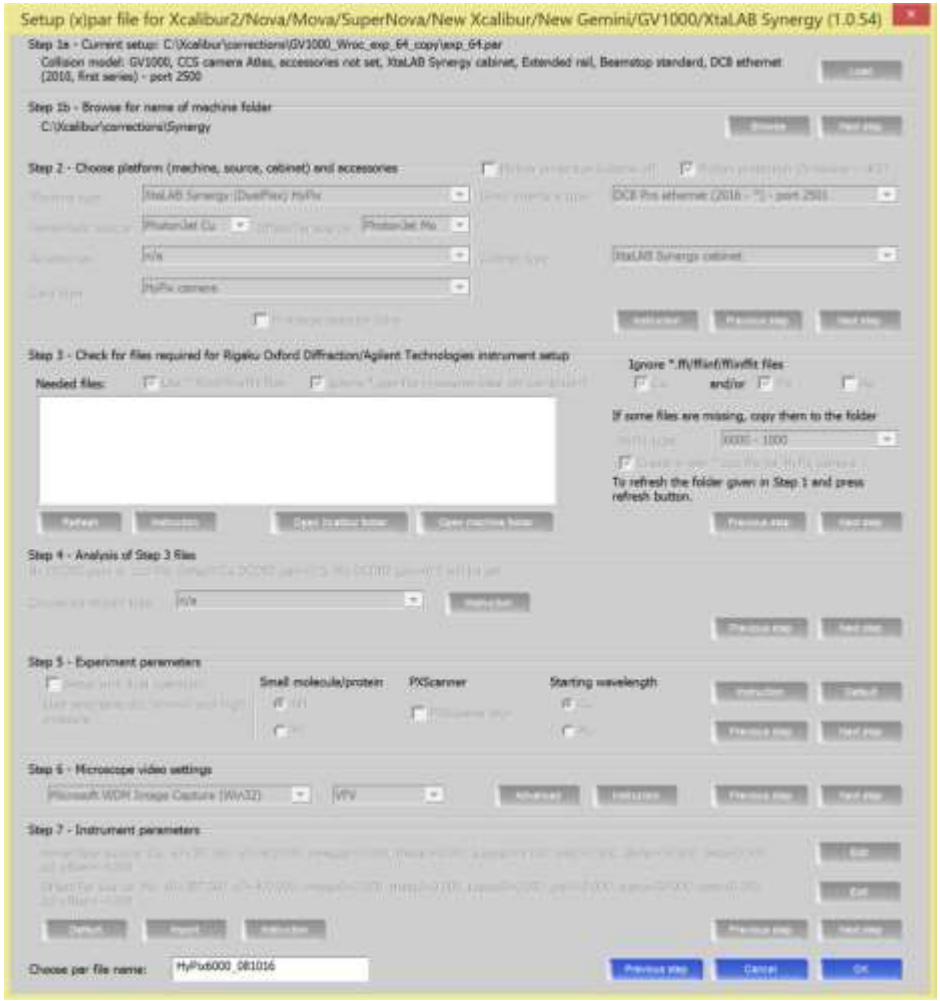
Workflow on inhouse instruments

Describe instrument



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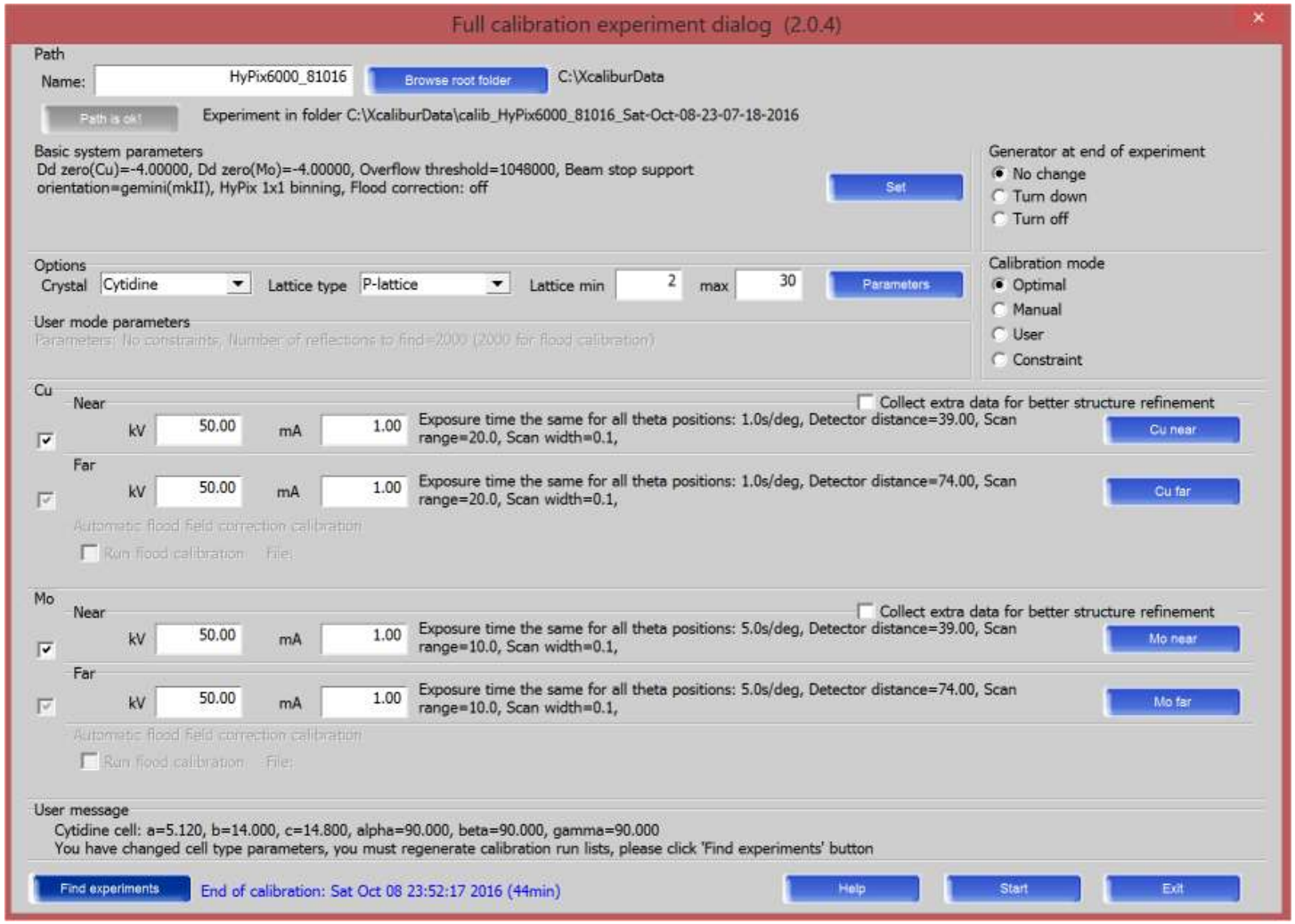
Workflow on in-house instruments

Run fully automatic calibration experiment describing fully the instrument at any distance



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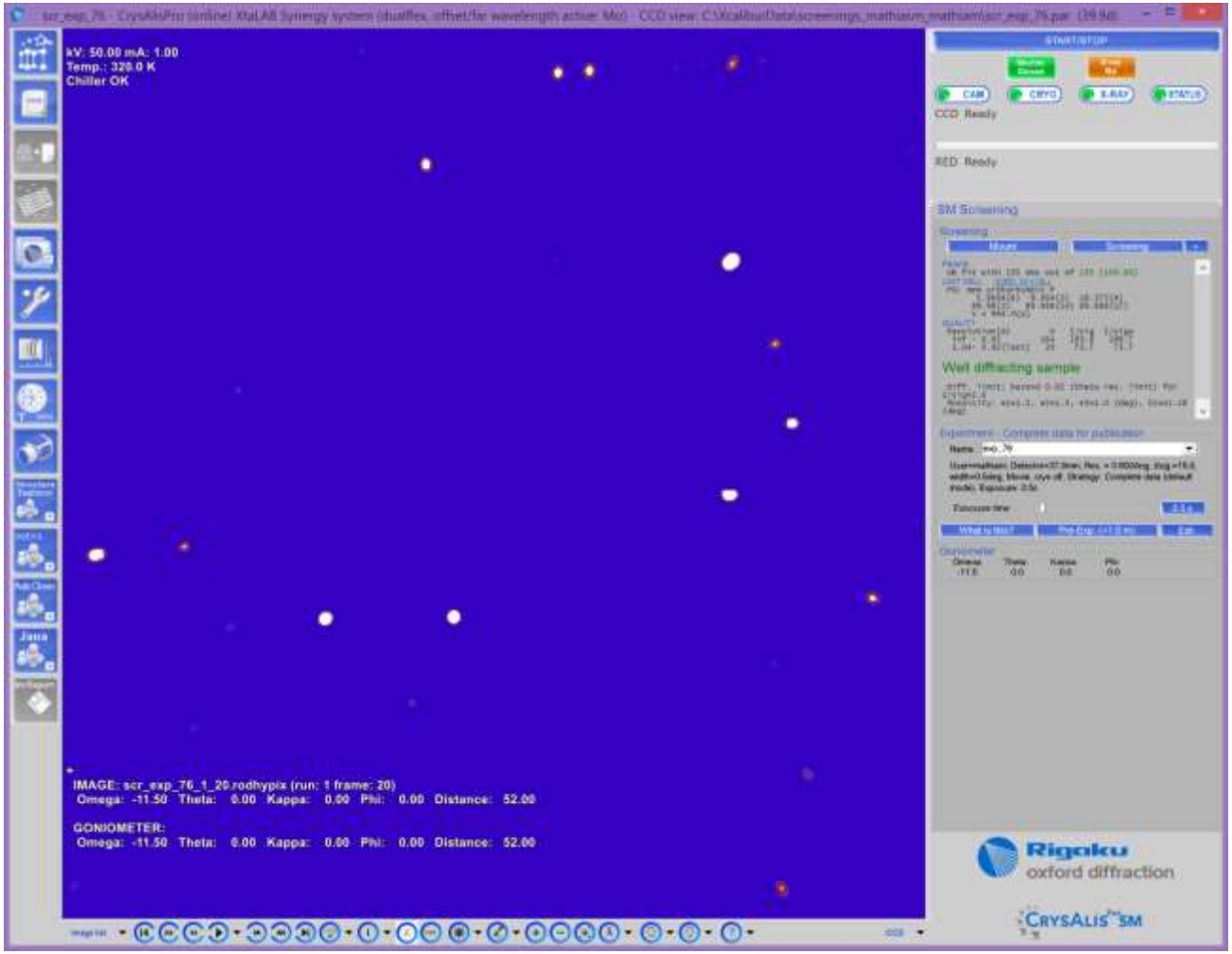
Workflow on in-house instruments

Run test data collection on standard sample



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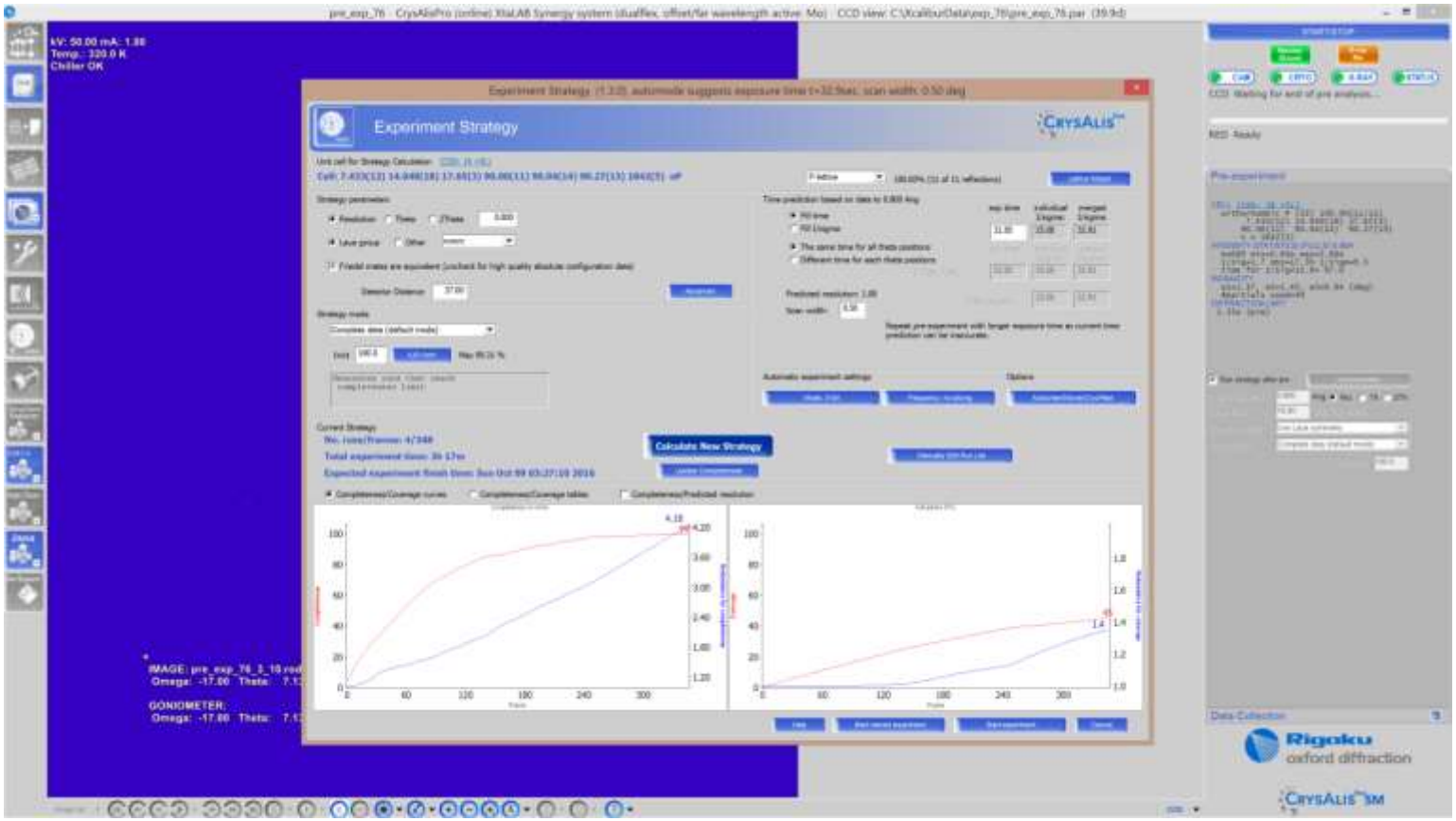
Workflow on in-house instruments

Run new experiment



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Import: Worse situation

- Depending on the format the instrument model is only known so-so.
- Rather than on a ‚Standard sample‘ the import is tried on something difficult.
- ‚Easy‘: Import of known formats
- ‚Complex‘: Esperanto import

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First meeting with the data set

- Install CrysAlisPro: this will install a tool called ‚CAPFrameView‘. You can inspect all known image formats.
- Use of a file inspection program: ‚Norton commander‘
- A rename tool.

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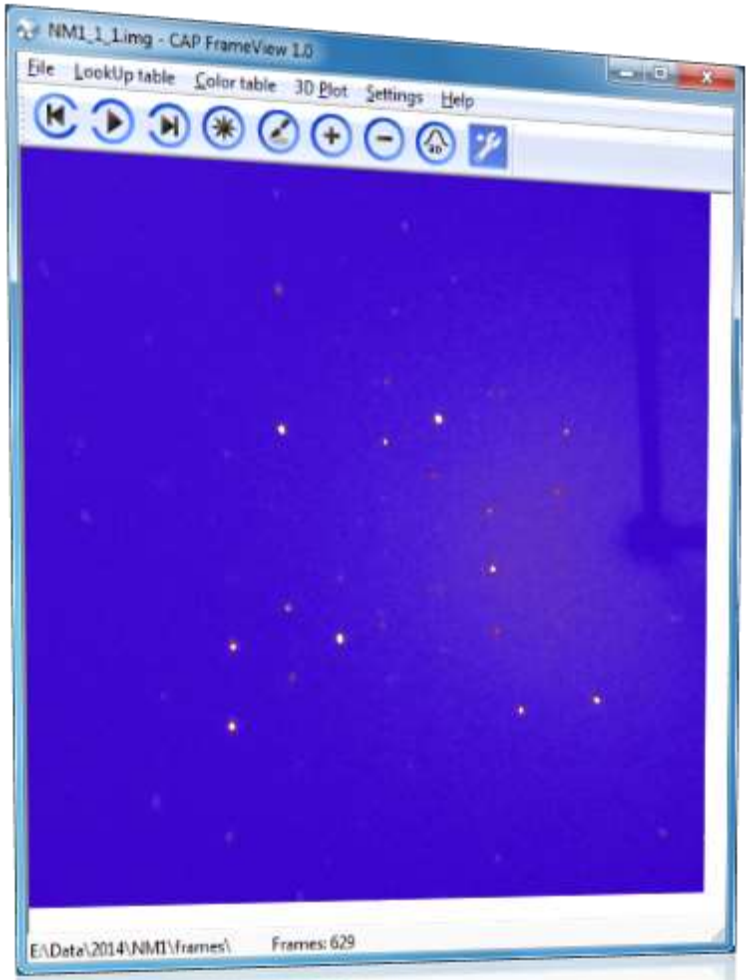
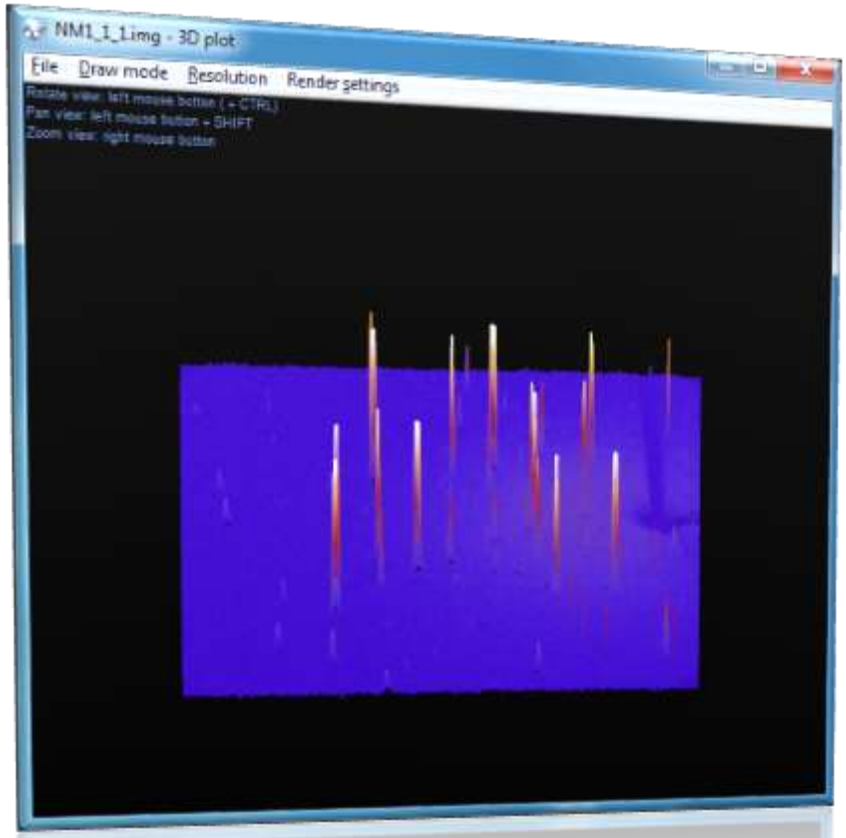
First meeting with the data set



Main window



3D Plot window

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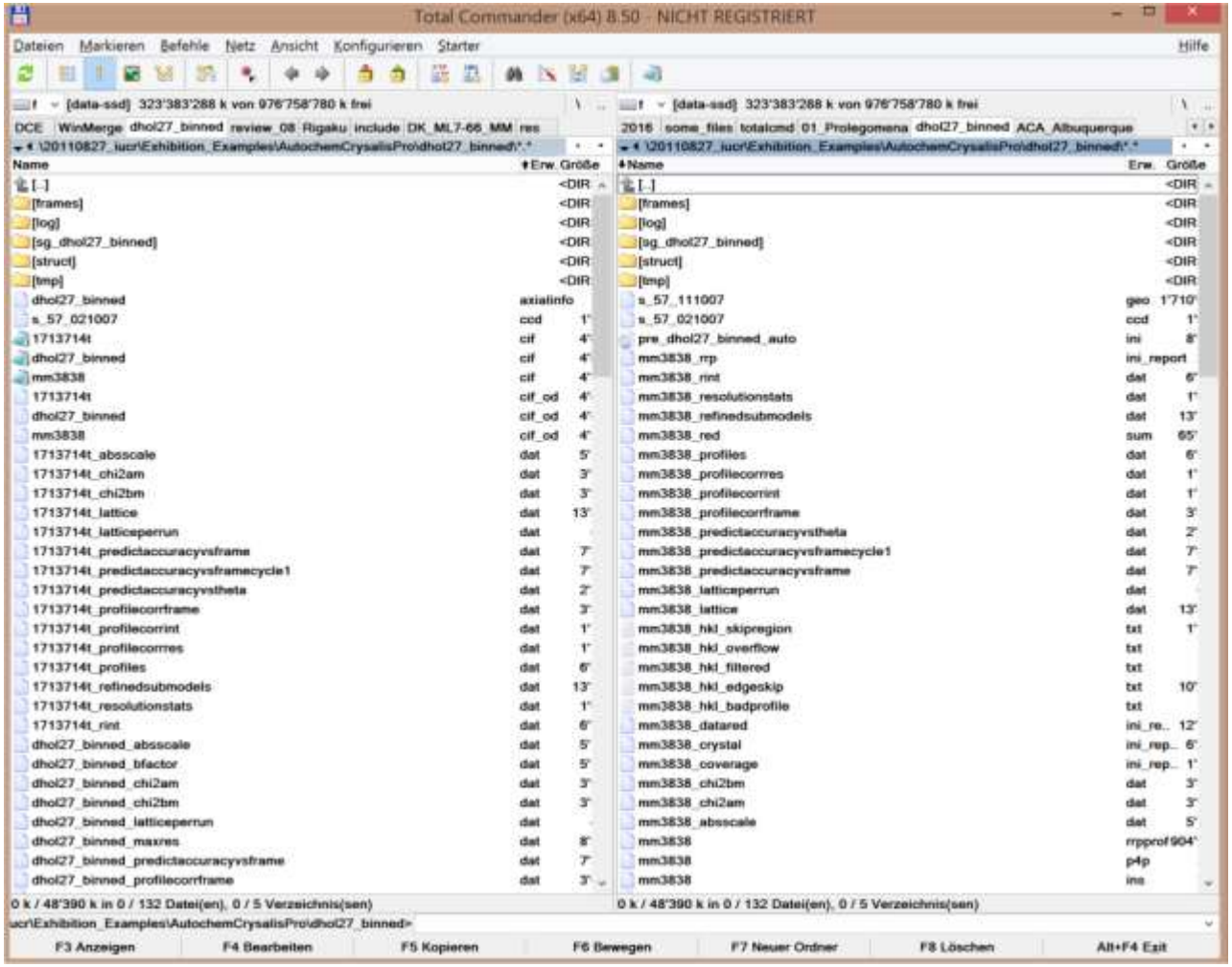
First meeting with the data set



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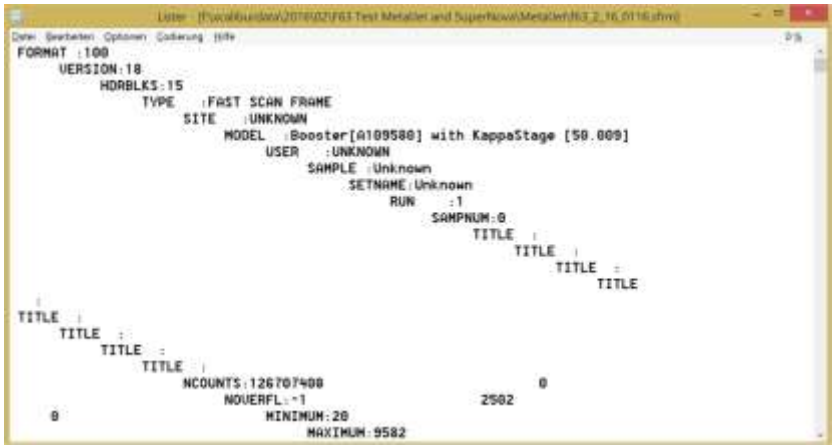
First meeting with the data set



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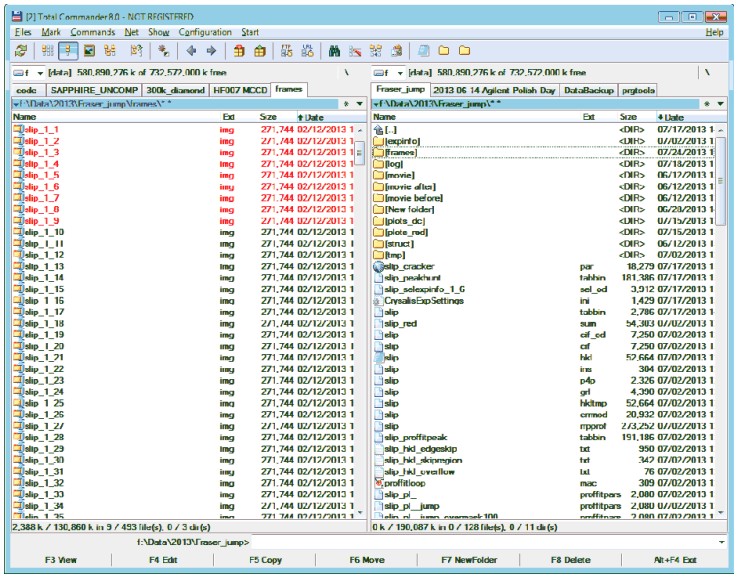
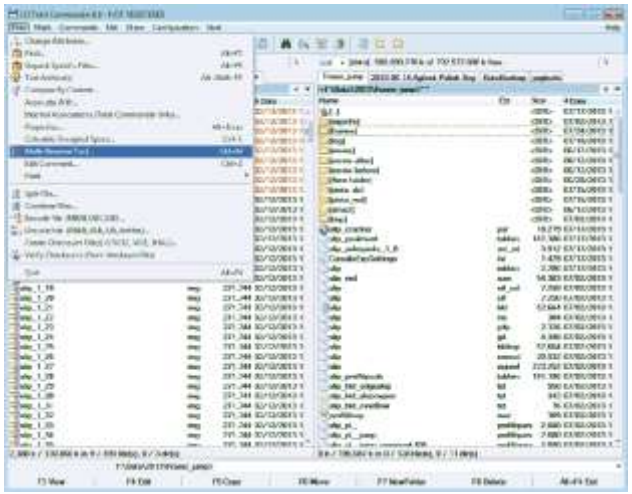
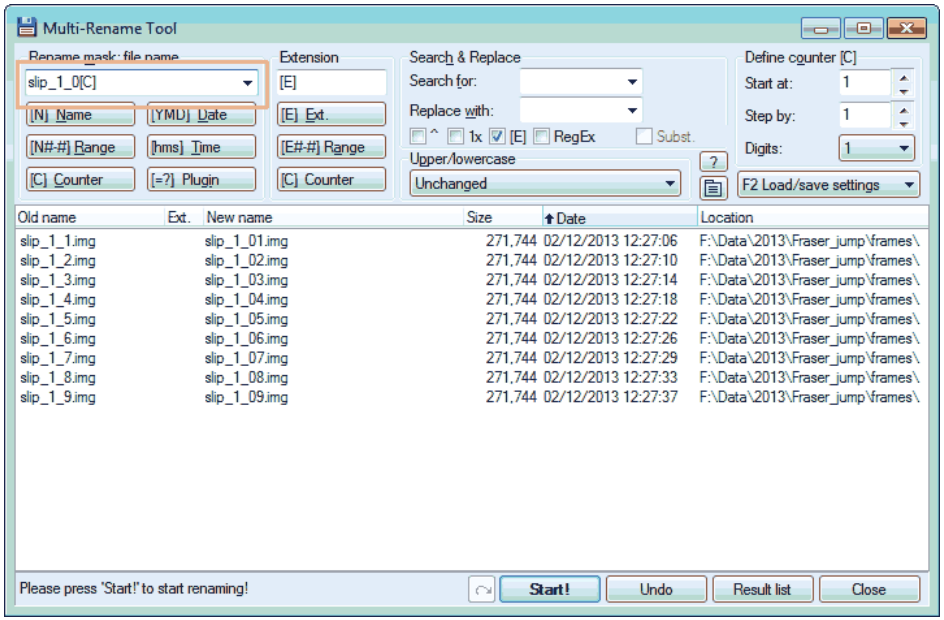
First meeting with the data set

rename







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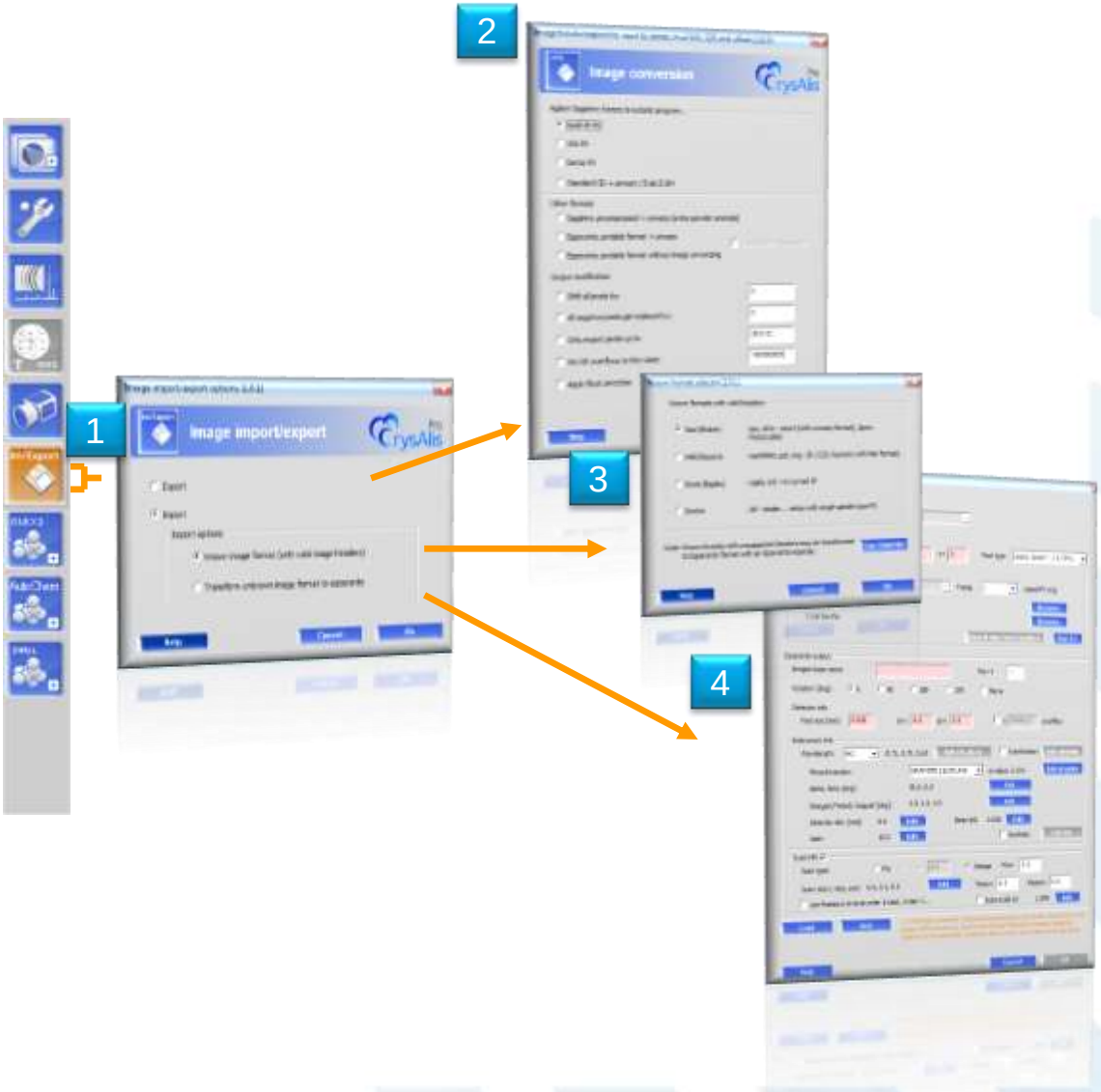
Import tools

1. Easier access to import/export options (on power toolbar).
2. Organized export options.
3. Importing external images on one clique (instead of typing commands).
4. Esperanto importer for non standard image types.



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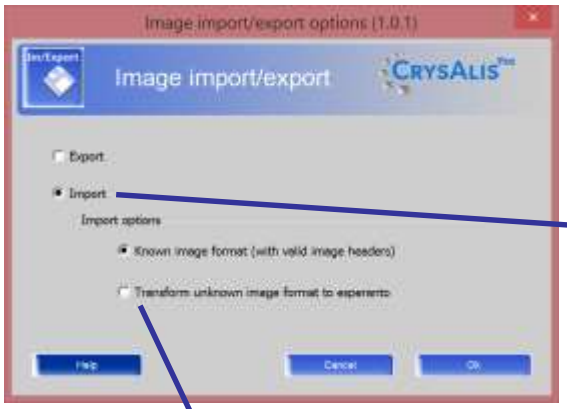
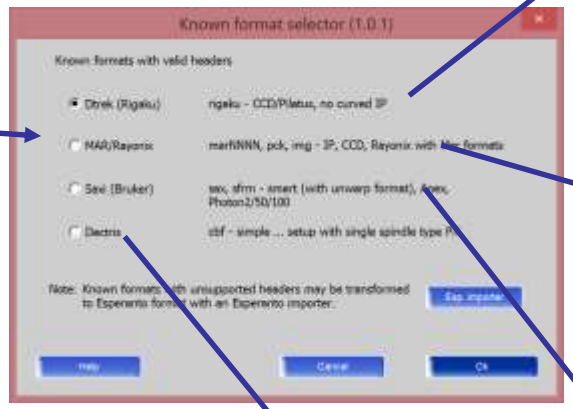
Known formats and esperanto





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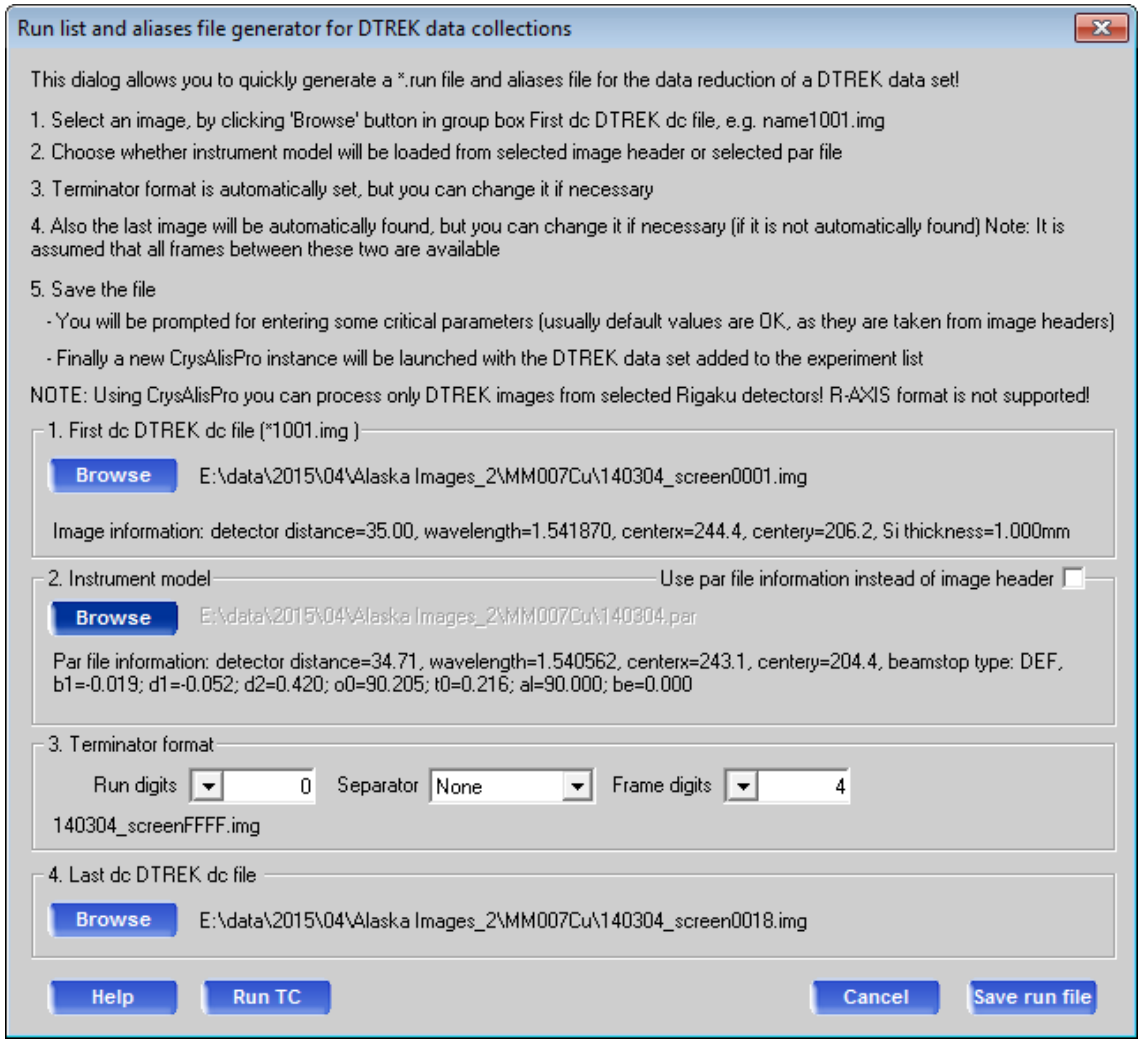
External Frame & File Formats

Rigaku – dtrek format



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Example: Apex data from ECM-Basel

- Handling of twin data…
- Dr. Daniel Kratzert (Freiburg, Germany) reduced a Bruker Apex2 twin with CAP and Saint.
- This presentation gives the workflow for importing and reducing Bruker data and handling twinning
- For the evaluation the forum version 38.43 was used.

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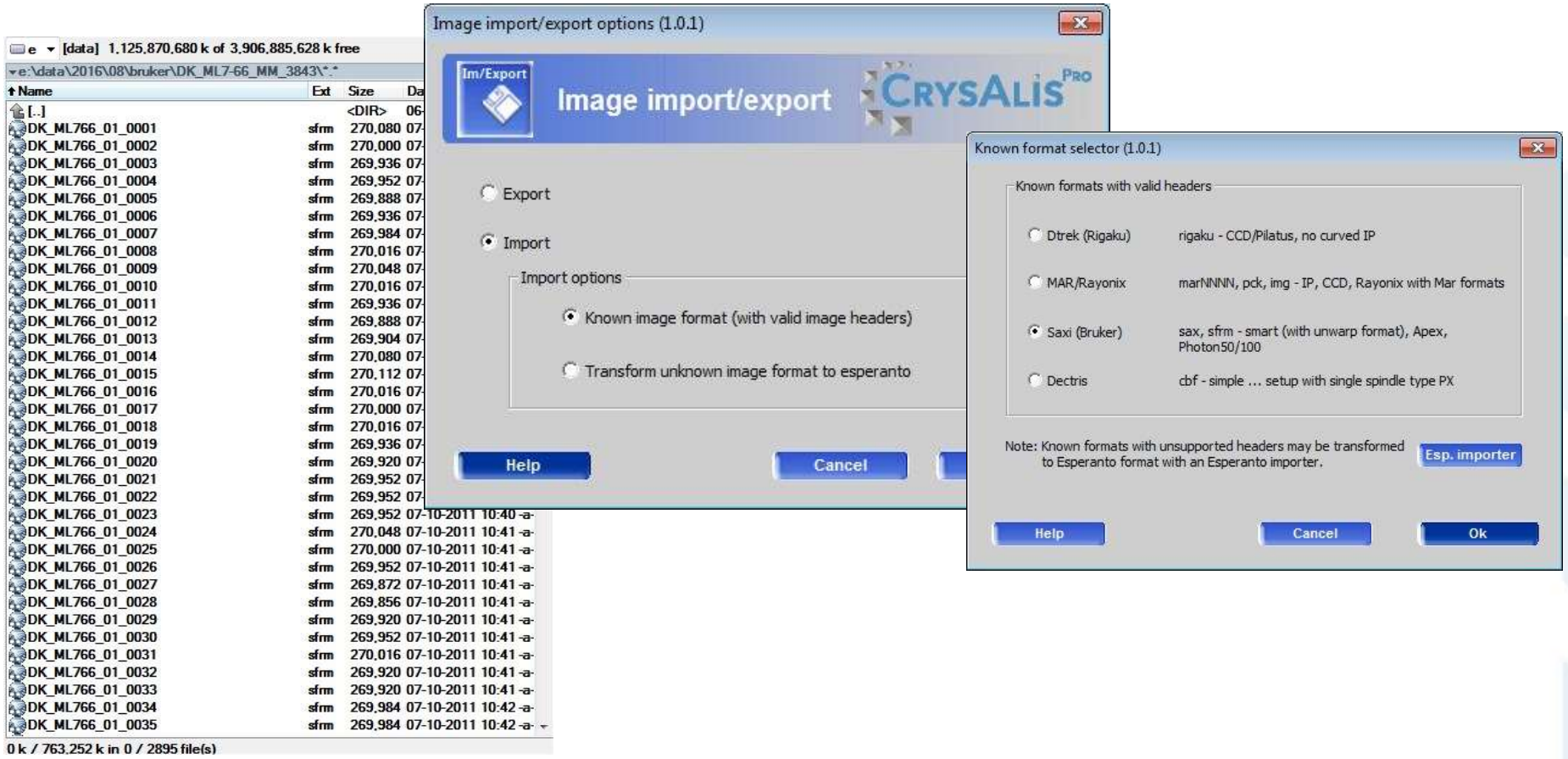
Data set import



- Open any existing experiment
- Import button

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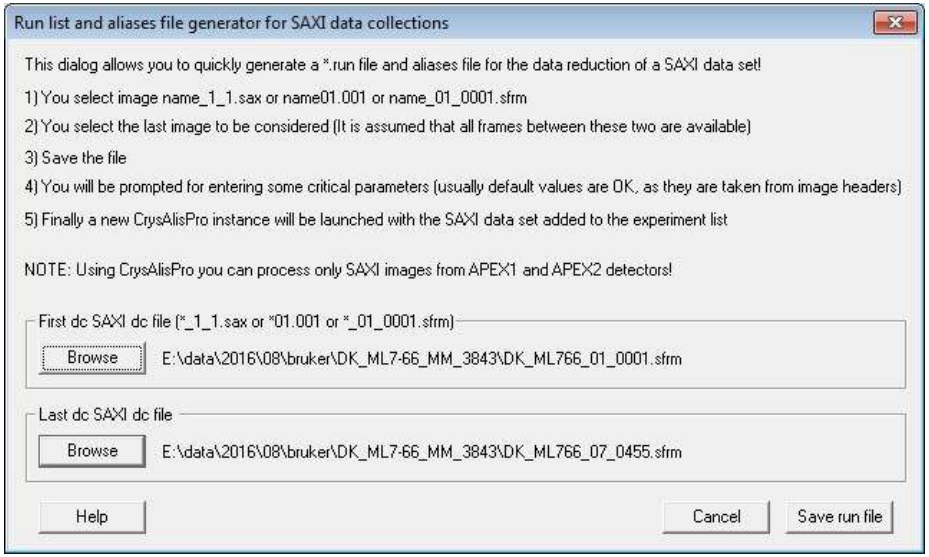
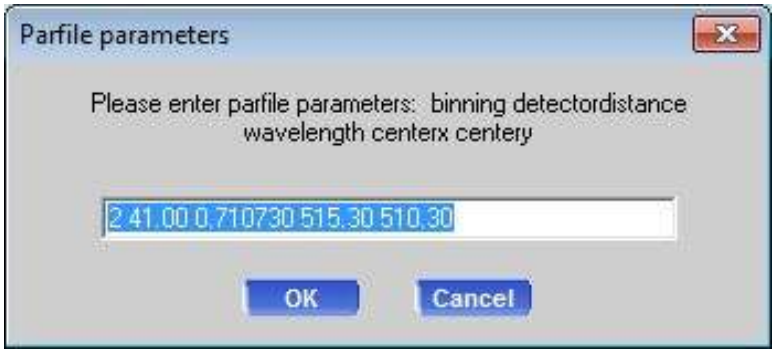
Data set import





- Open any existing experiment
- Import button

Data set facts

- Mo, Iμs, no Si filter showoing 3λ effect
- Frame width: 0.4, correlated ? Frames

CrysAlisPro run list data

Data collection mode: correlated
Total number of frames:2889 (scan: 2889, reference: 0)
Disk space: 763.79Mb
Approximate data collection time (h:min): 10:55

#	t	start	end	width	exposure		speed-rat	omega	theta	kappa	phi	# to do	# done
1	o	1.386	184.186	0.400	5.000+	5.000	0.000	-	30.000	73.926	-0.814	456	456
2	o	-11.114	171.686	0.400	3.000+	3.000	0.000	-	17.500	73.926	4.186	456	456
3	o	21.376	163.775	0.400	3.000+	3.000	0.000	-	10.000	73.926	86.686	356	356
4	o	21.786	174.186	0.400	3.000+	3.000	0.000	-	20.000	73.926	-35.816	380	380
5	o	-28.114	126.686	0.400	5.000+	5.000	0.000	-	-27.500	73.926	11.685	386	386
6	o	18.386	179.186	0.400	4.000+	4.000	0.000	-	25.000	73.926	9.184	401	401
7	o	-7.815	174.186	0.400	3.000+	3.000	0.000	-	20.000	73.926	-60.814	454	454

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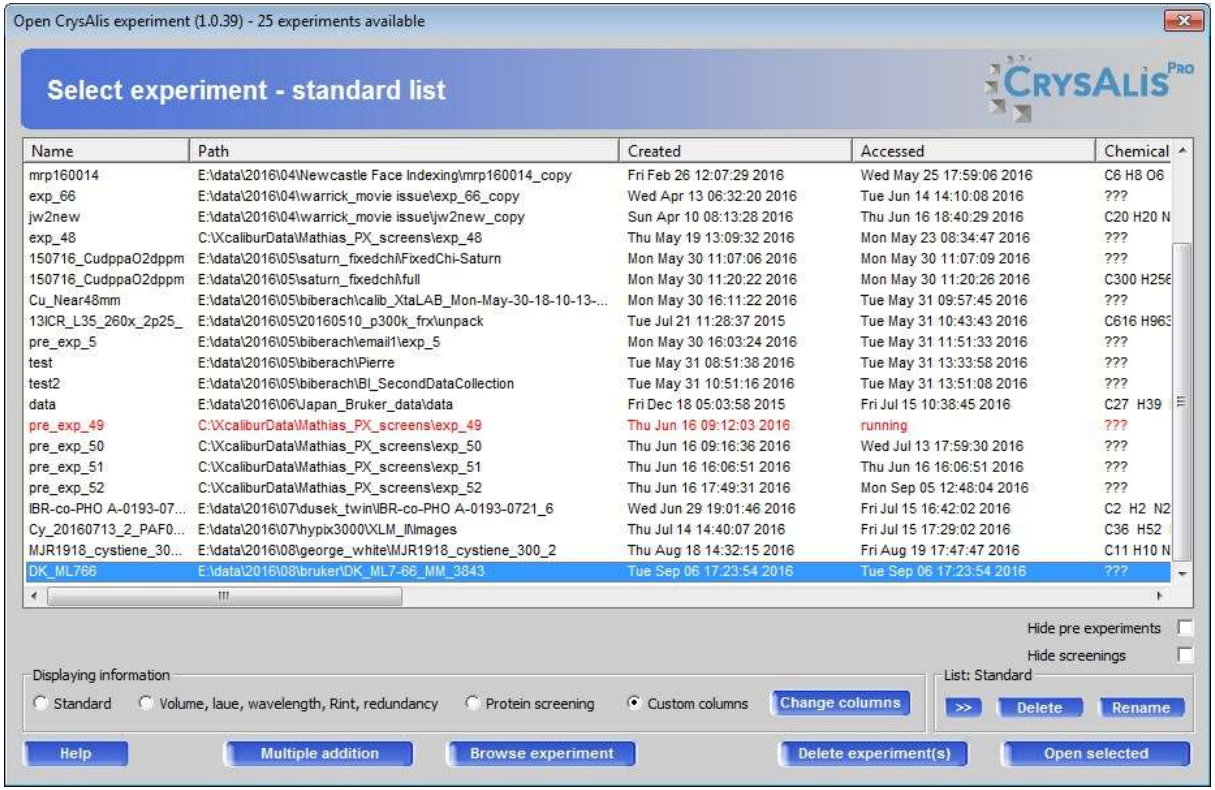
First opening of the data set

- Select SM/PX nature



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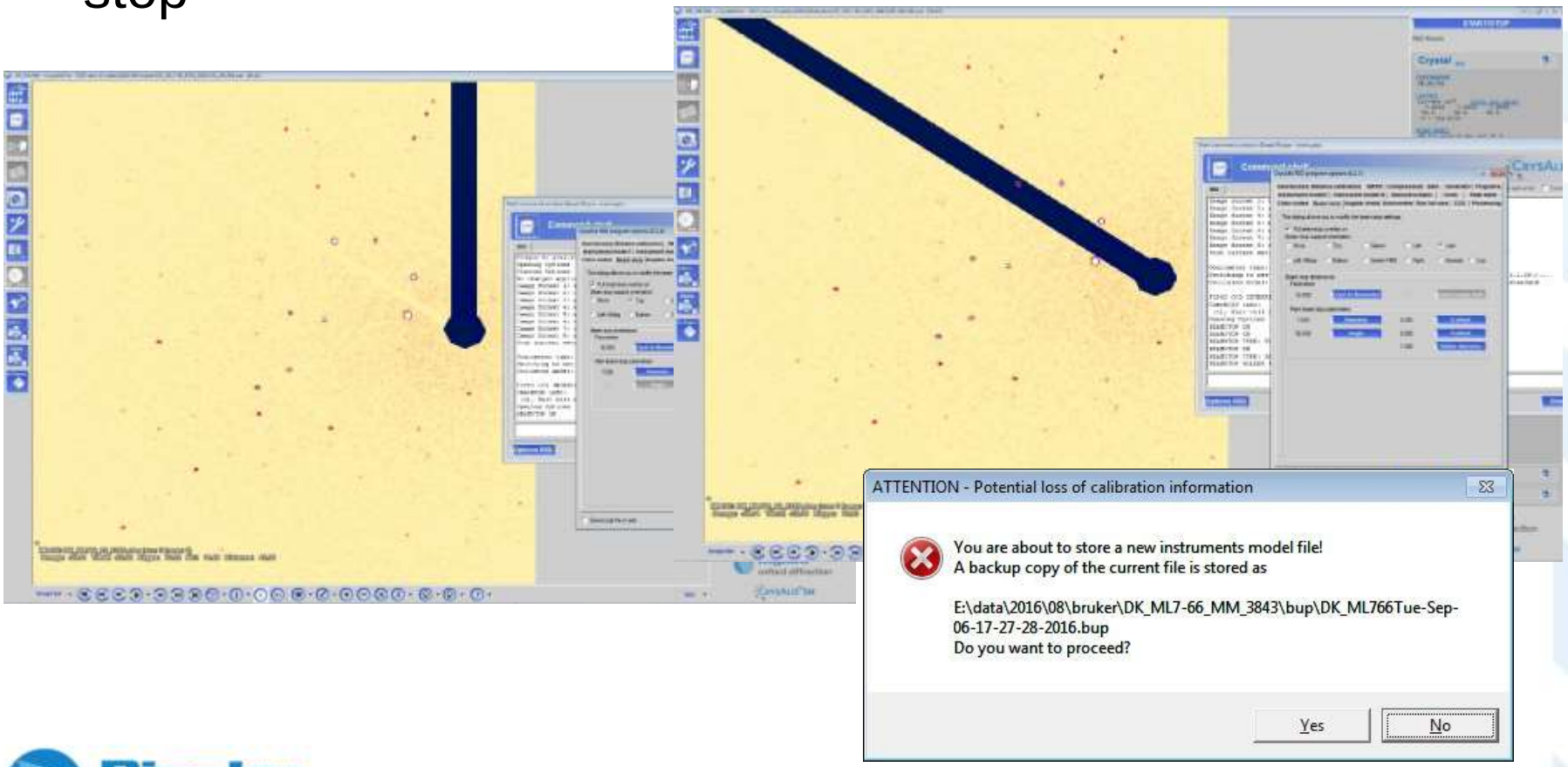
Set the beam stop

- Apex system sometimes use a user angle for the beam stop



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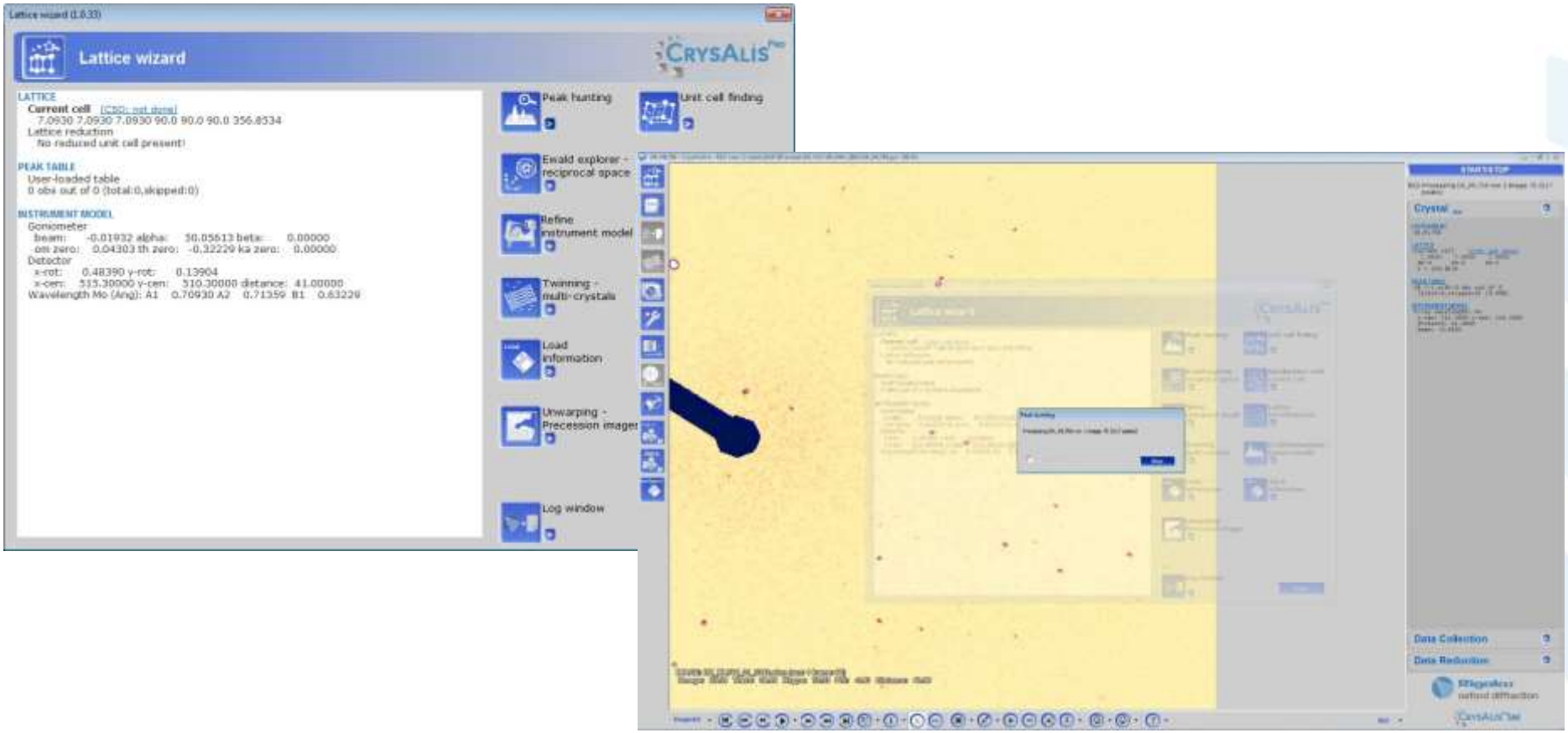
First peak hunting

- Use default



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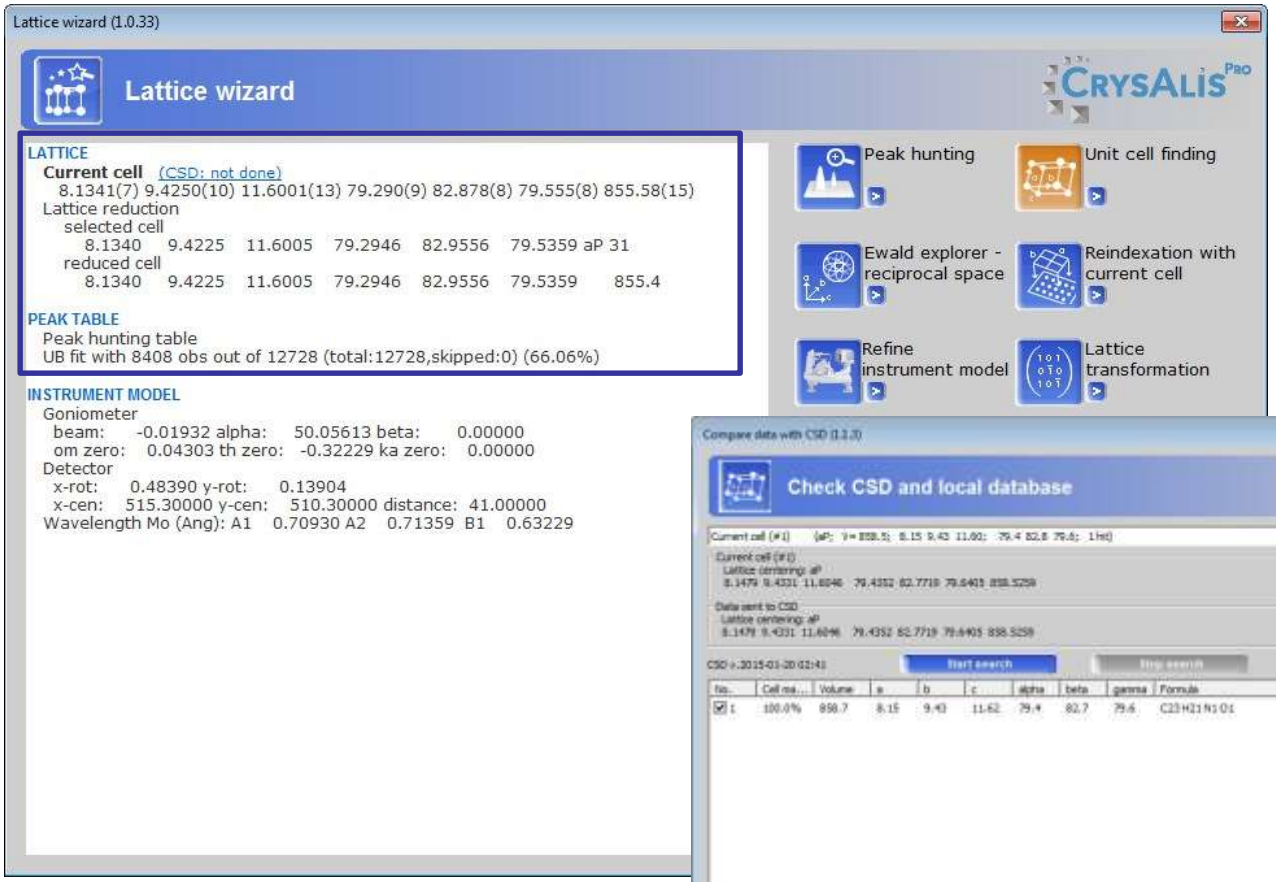
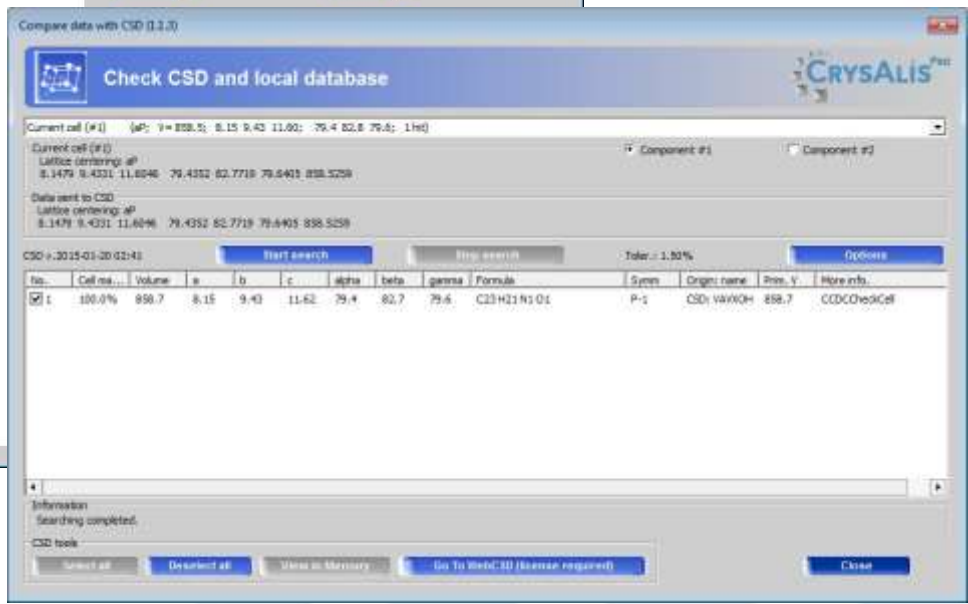
Automatic unit cell finding

- Use default, 66% indexed, in spite of slightly off model





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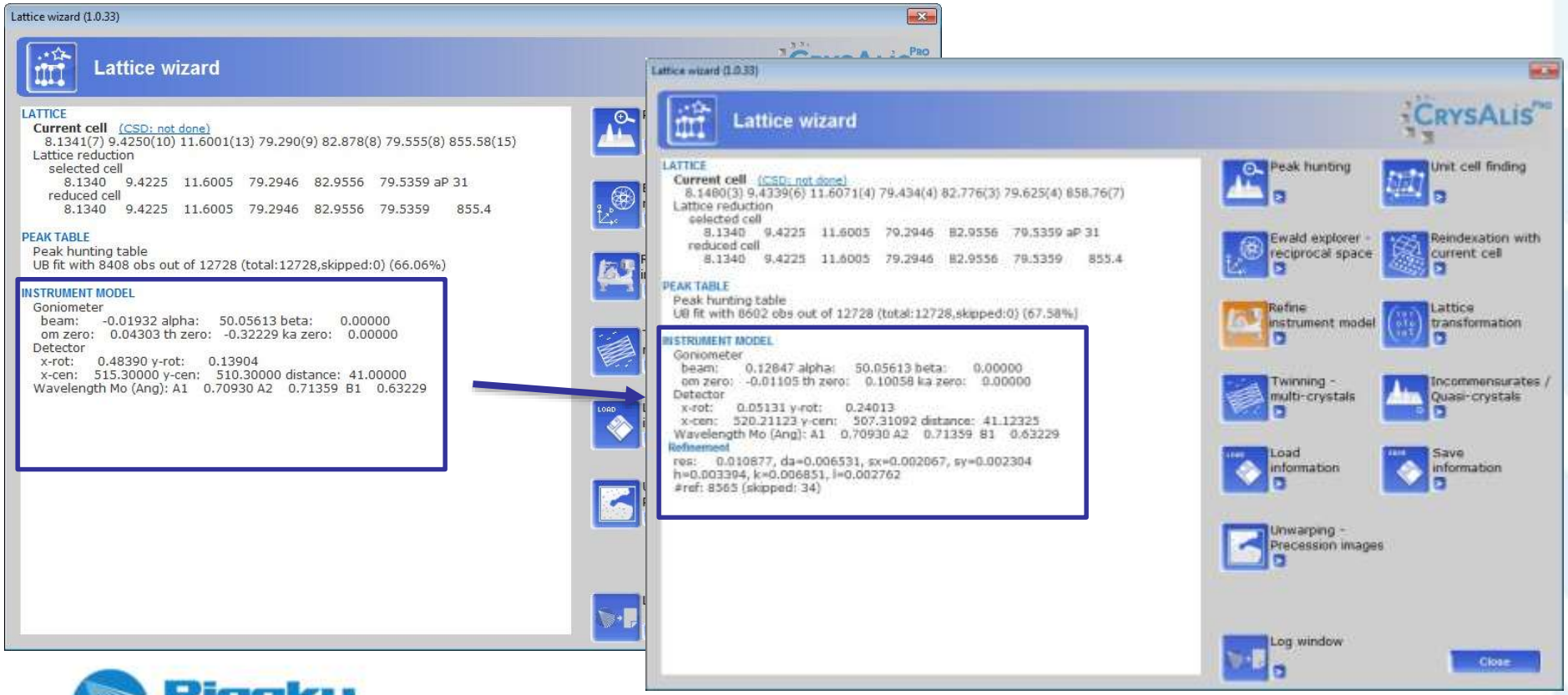
First instrument model refinement

- The header info is not precise. Refine on full data.
- Use default



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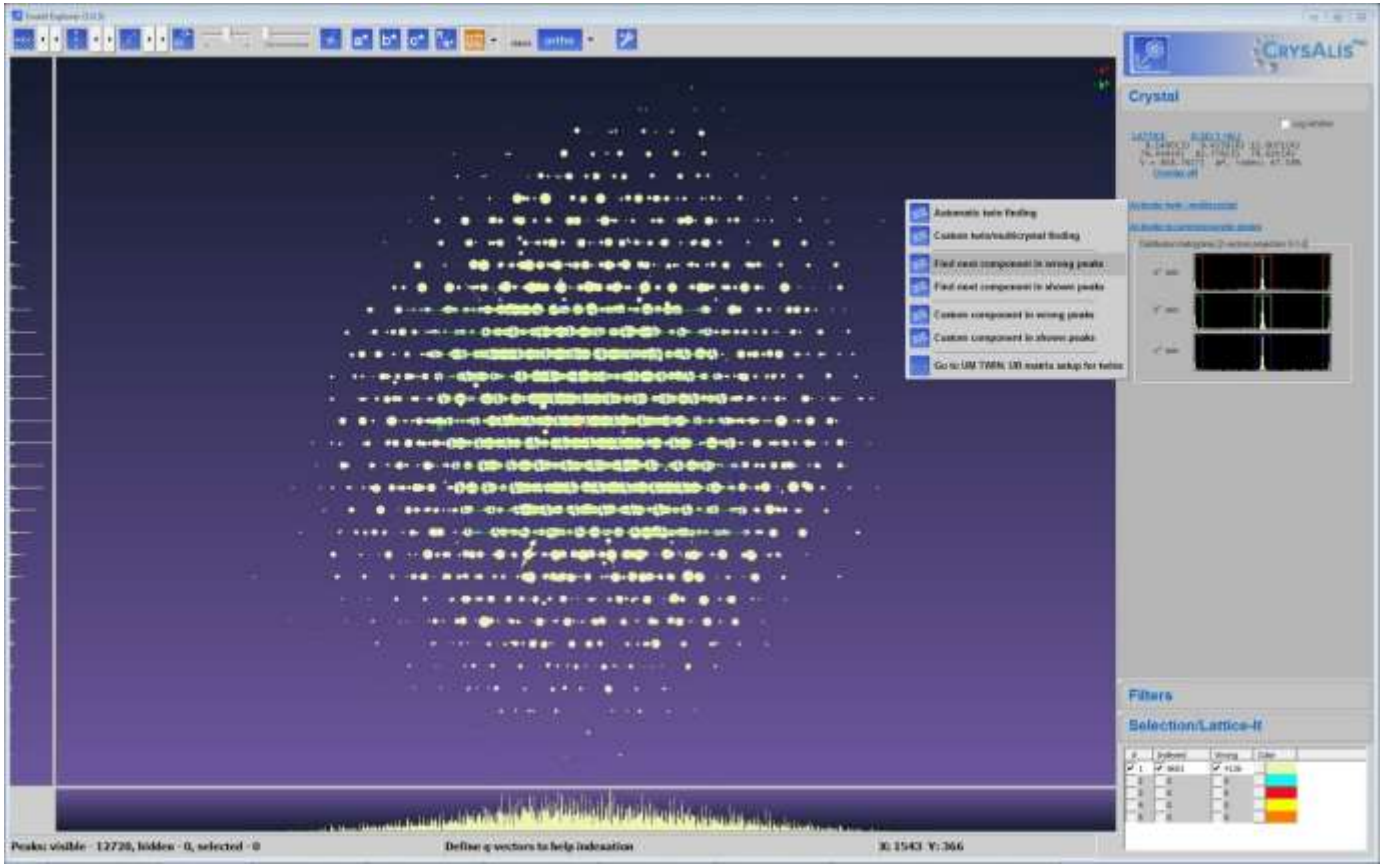
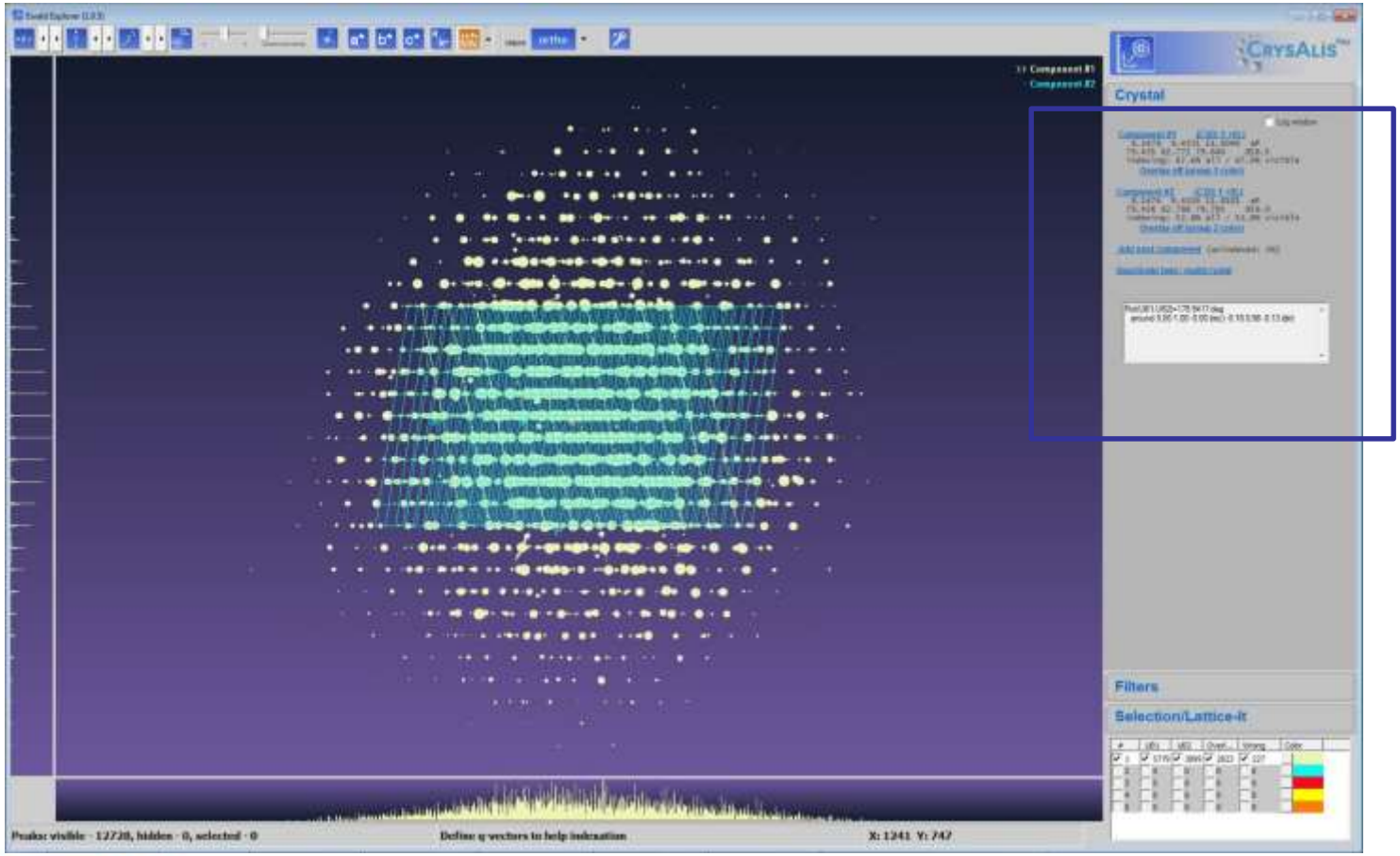
Use EwaldPro to find the twin

- Find next component in wrong peaks



Use EwaldPro to find the twin

- Easy: 180 deg rotation twin



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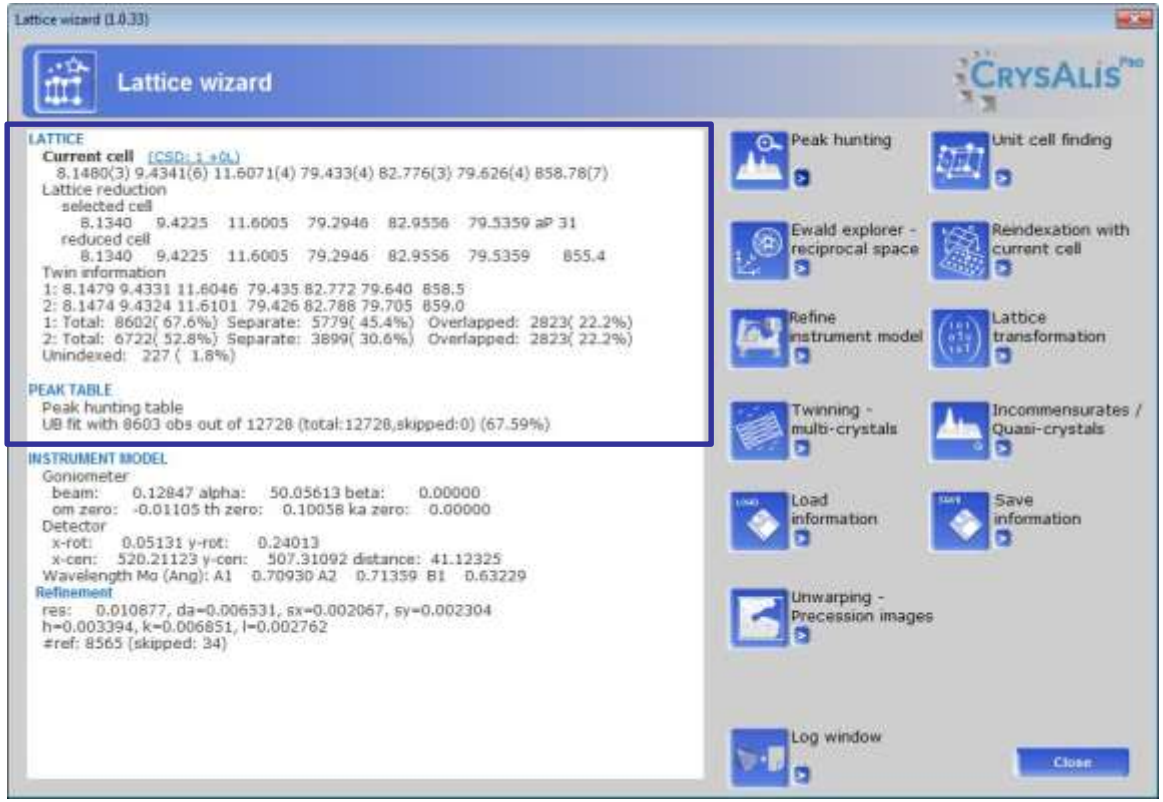
Use EwaldPro to find the twin

- Back to lattice wizard…



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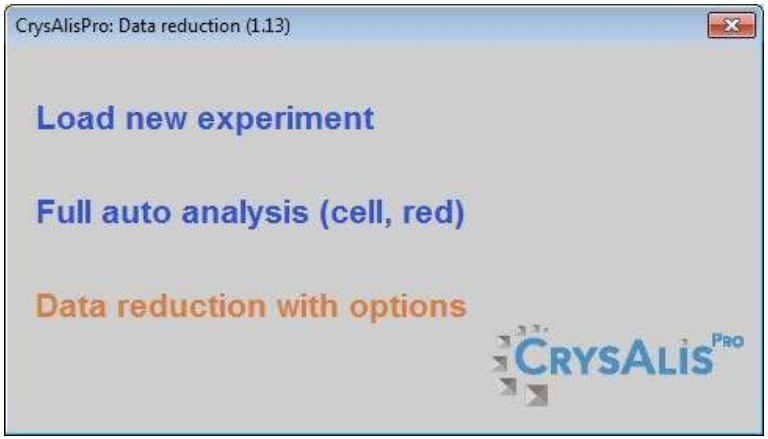
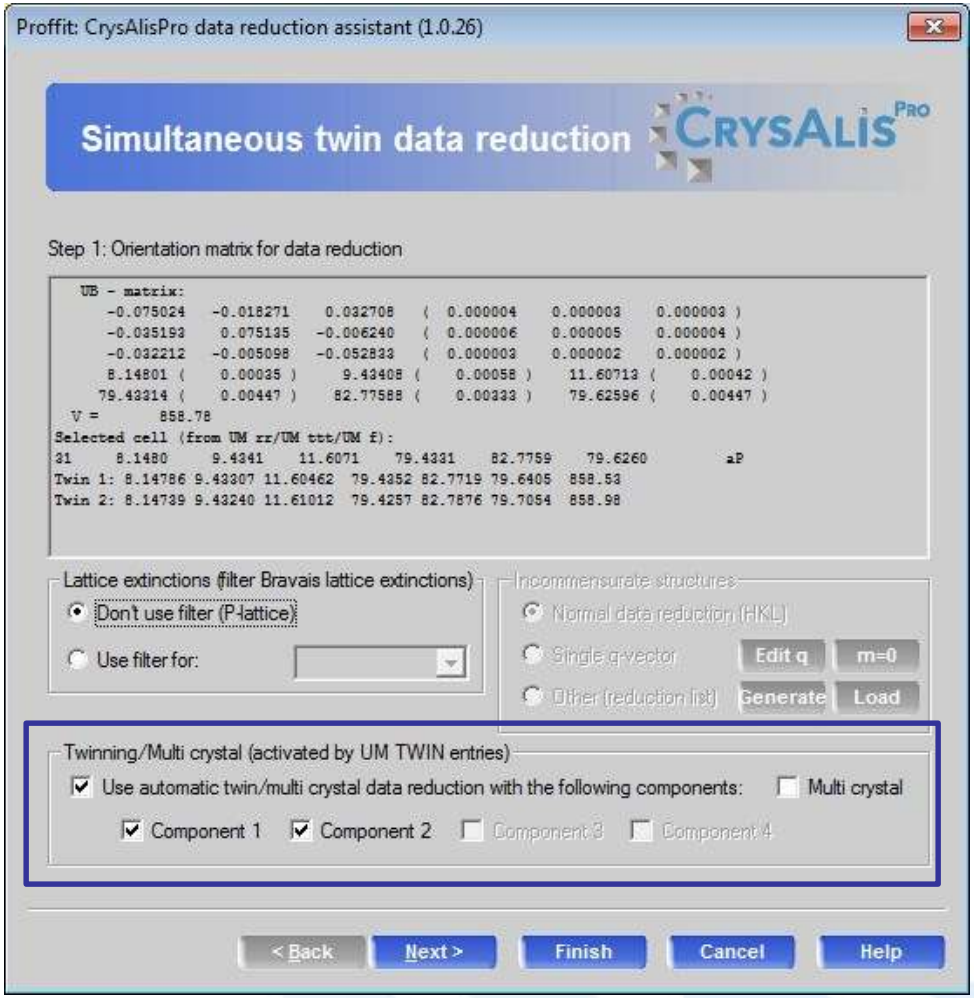
Do twin data reduction

- Run the data reduction wizard. Twin reduction auto set…





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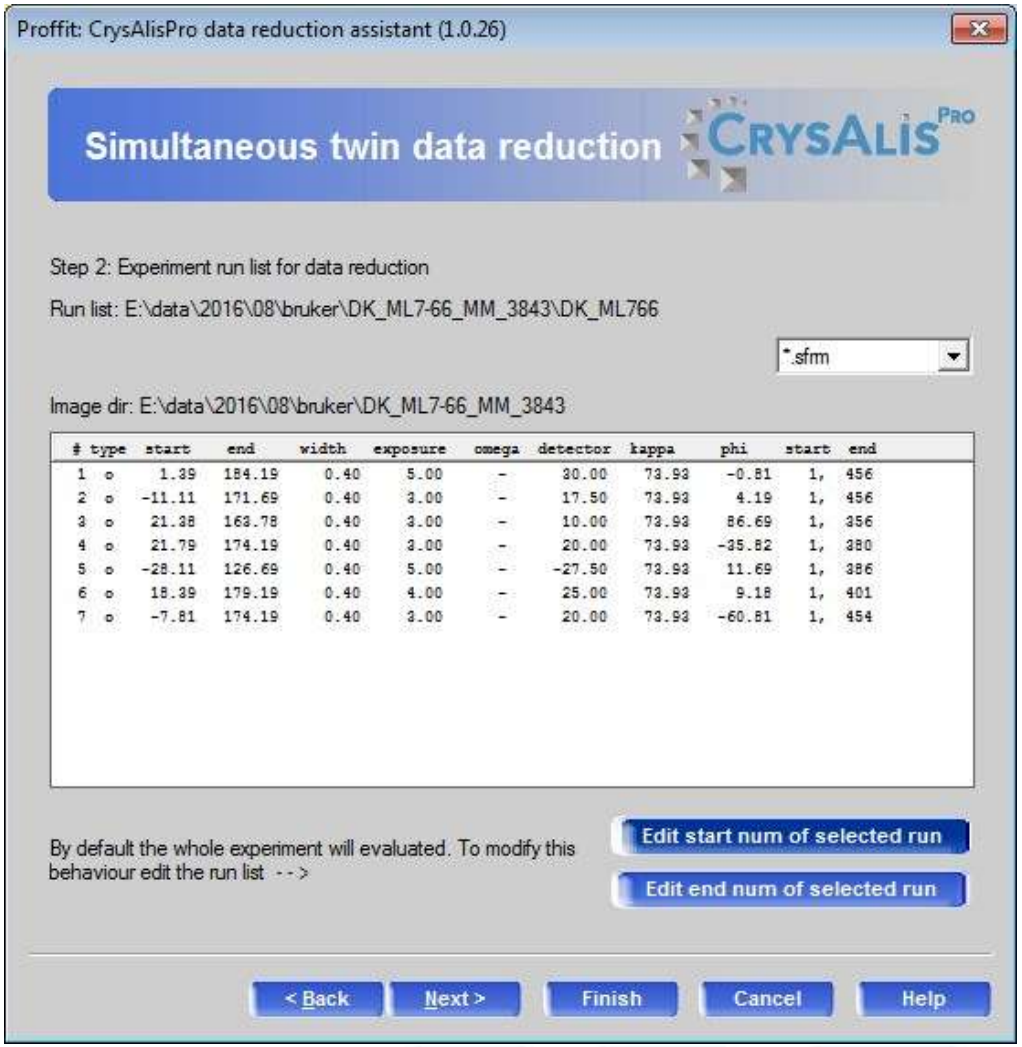
Do twin data reduction

- Accept the run list



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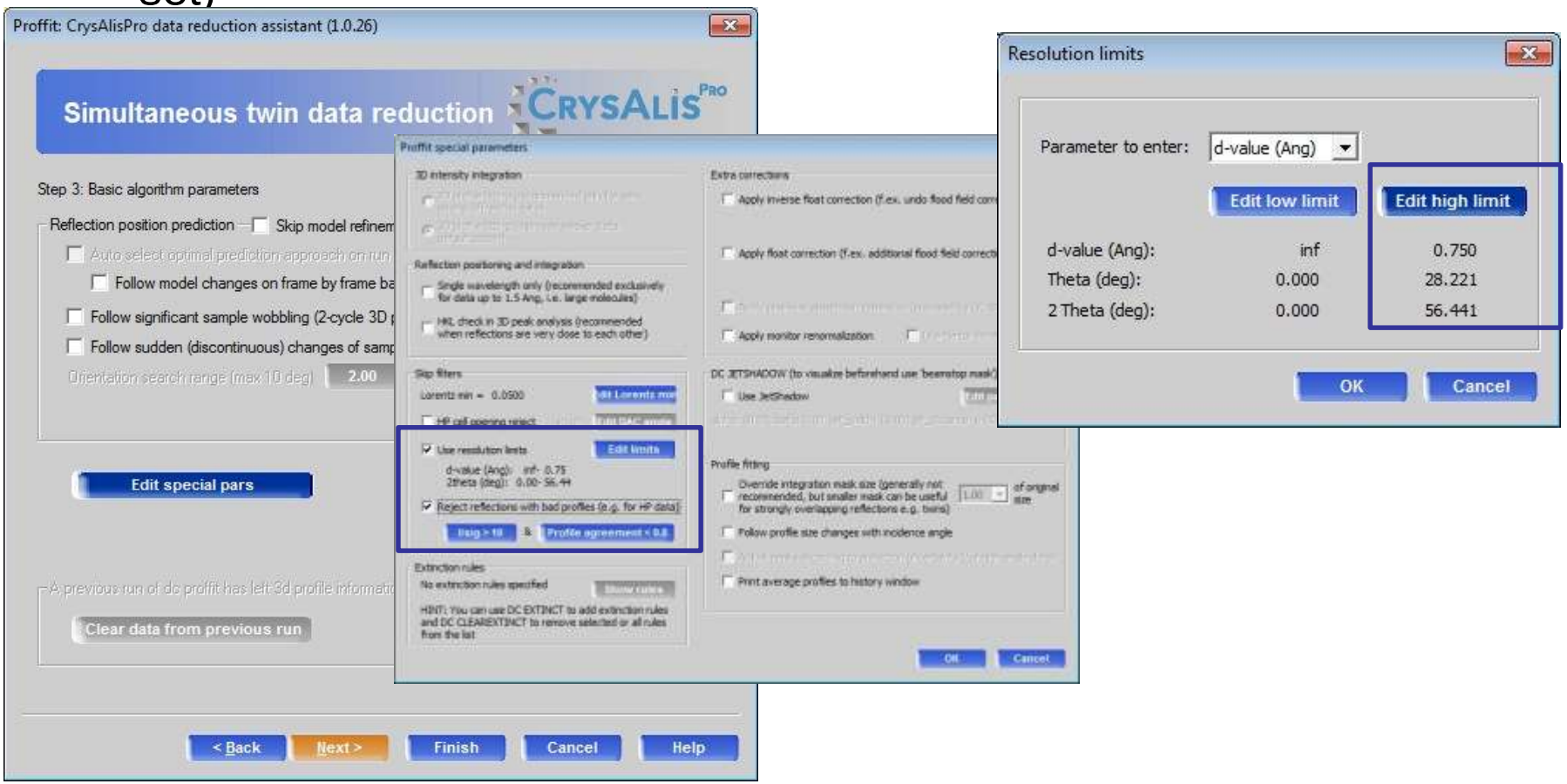
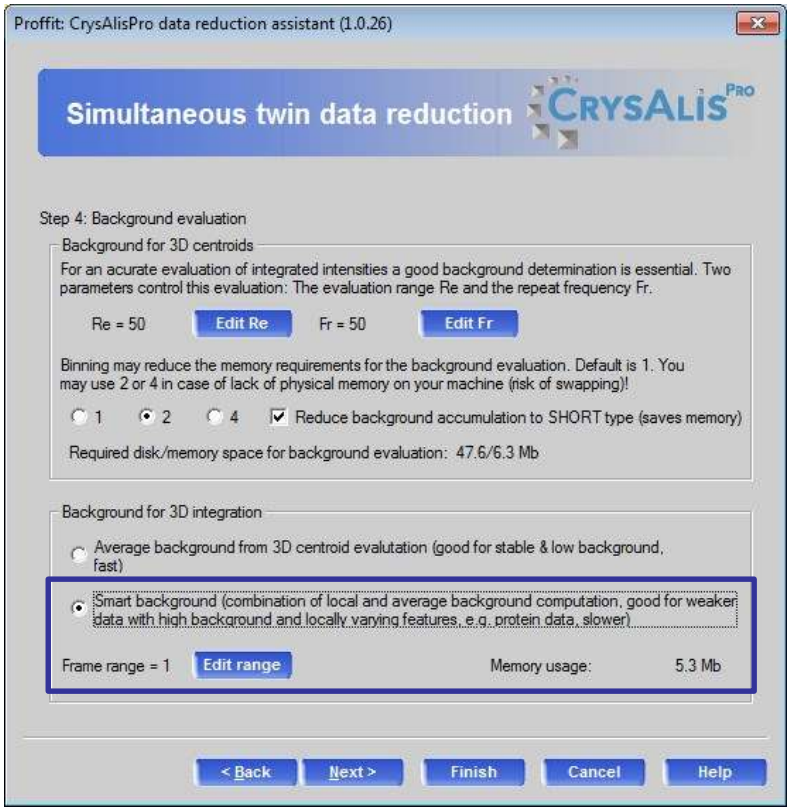
Do twin data reduction

- Special pars: All default; Limit the data to 0.75Ang (as done in the B set)



Do twin data reduction

- Background: Smart background



This is the most critical for the data set: It seems that the Apex detector has unstable background, thus introducing a bias on the average background method. Such behavior is also seen with other detectors where CAP uses by default Smart background.

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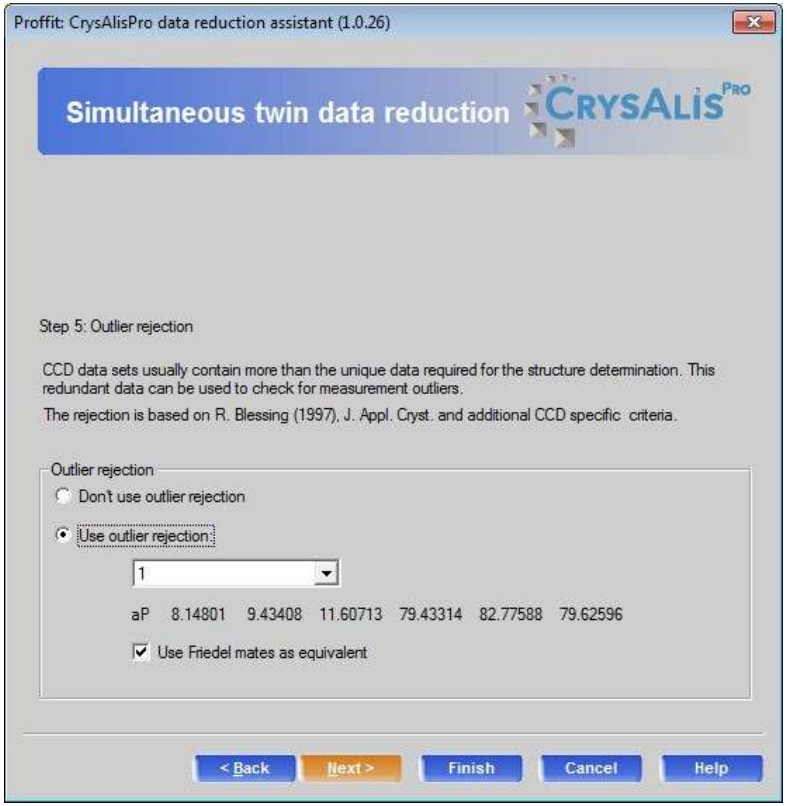
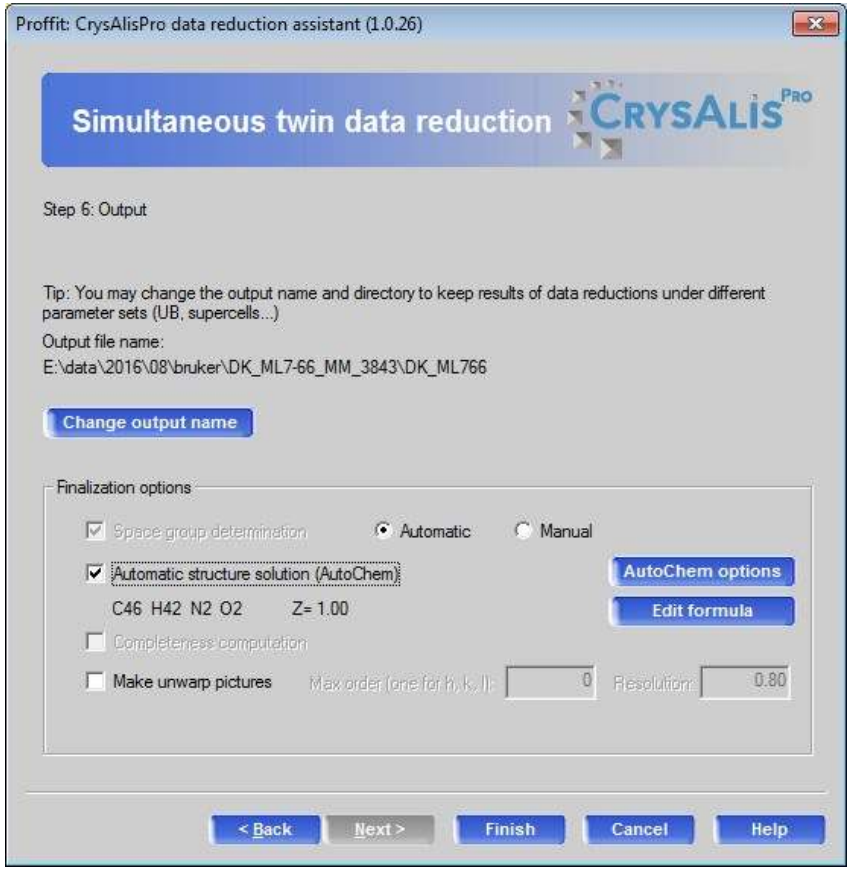
Do twin data reduction

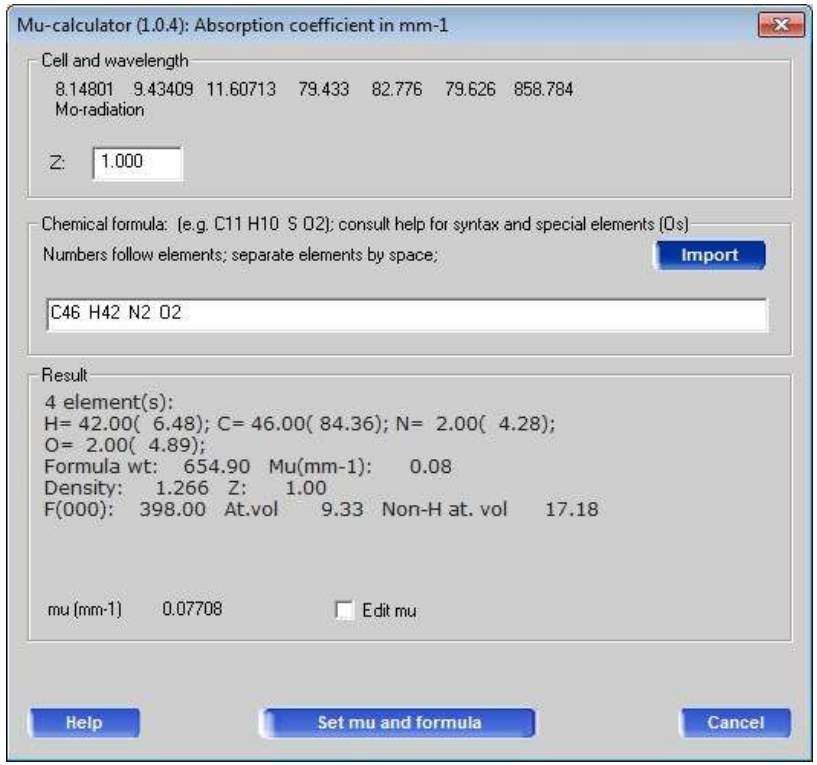
- Automatic outlier rejection: default



Do twin data reduction

- Chem. formula imported for AutoChem





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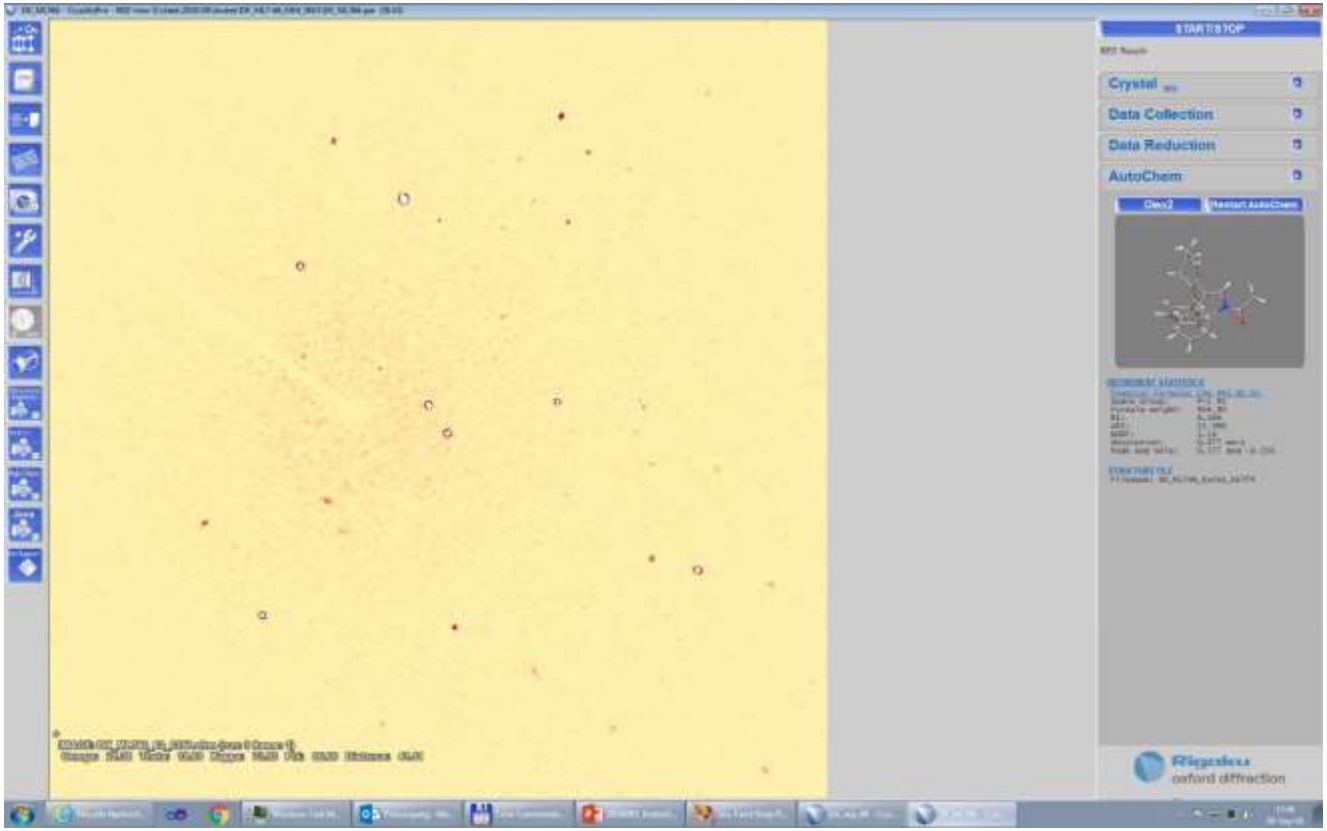
Automatic result

- Auto: based on all hklf4 data.



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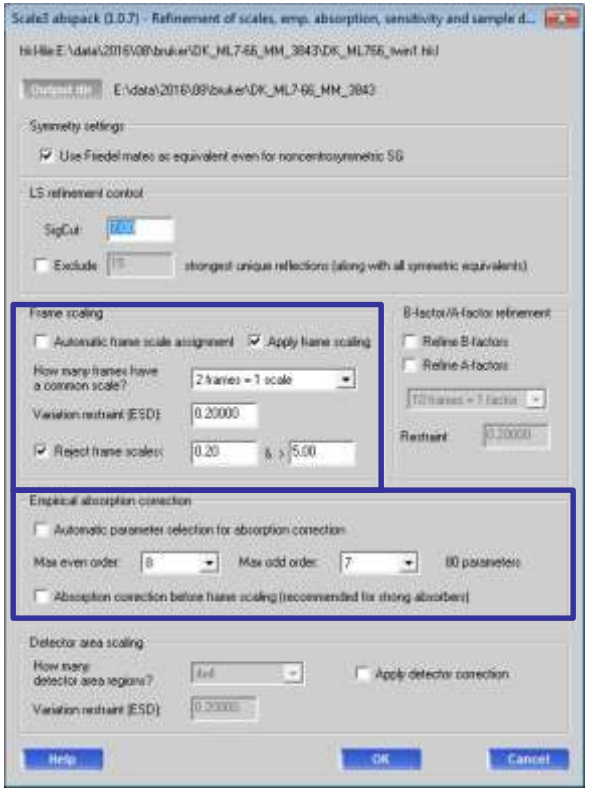
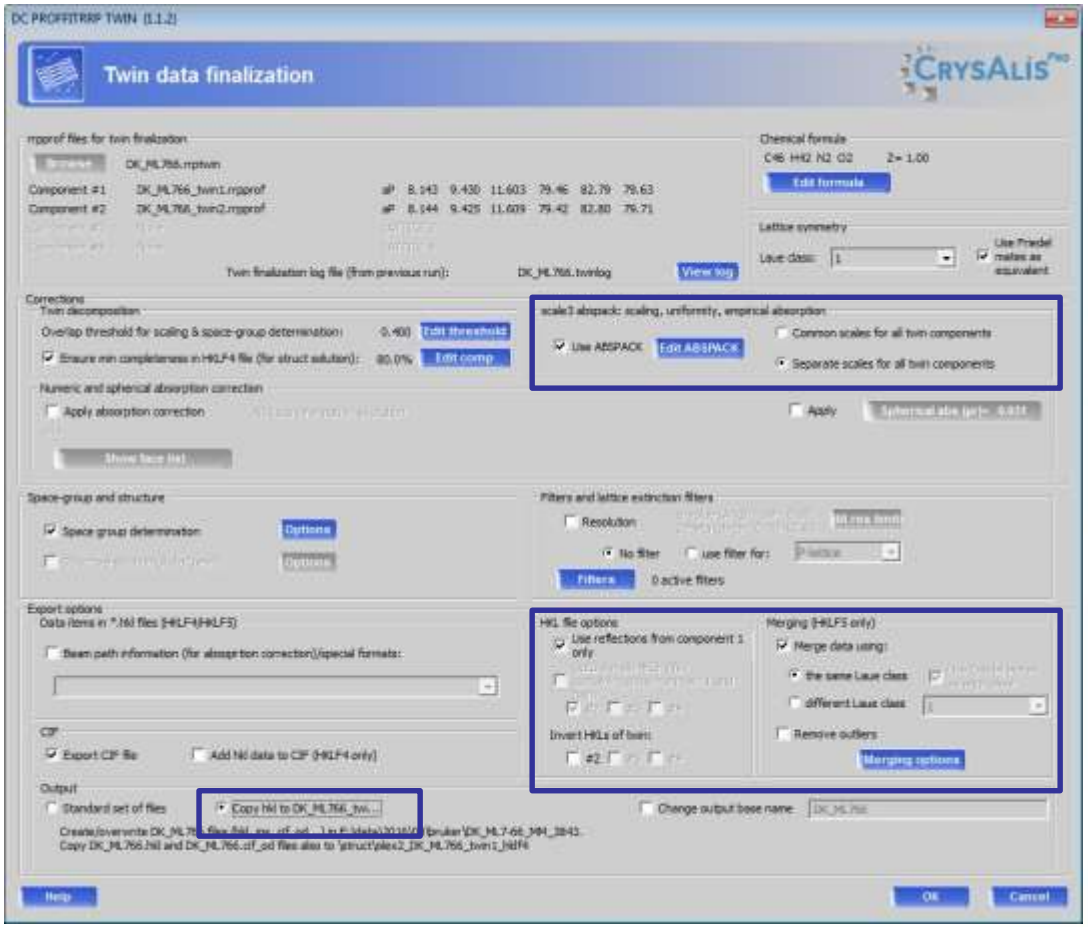
Tuning your result

- Tuning means what kind of scaling is used and what reflection classes are in the final hklf4 and 5 files





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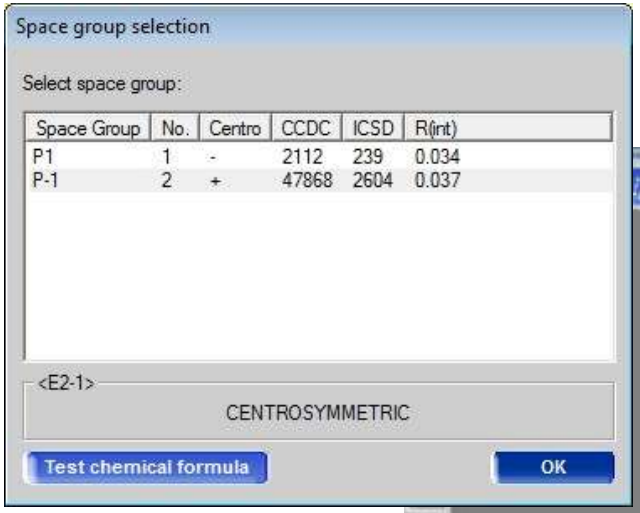
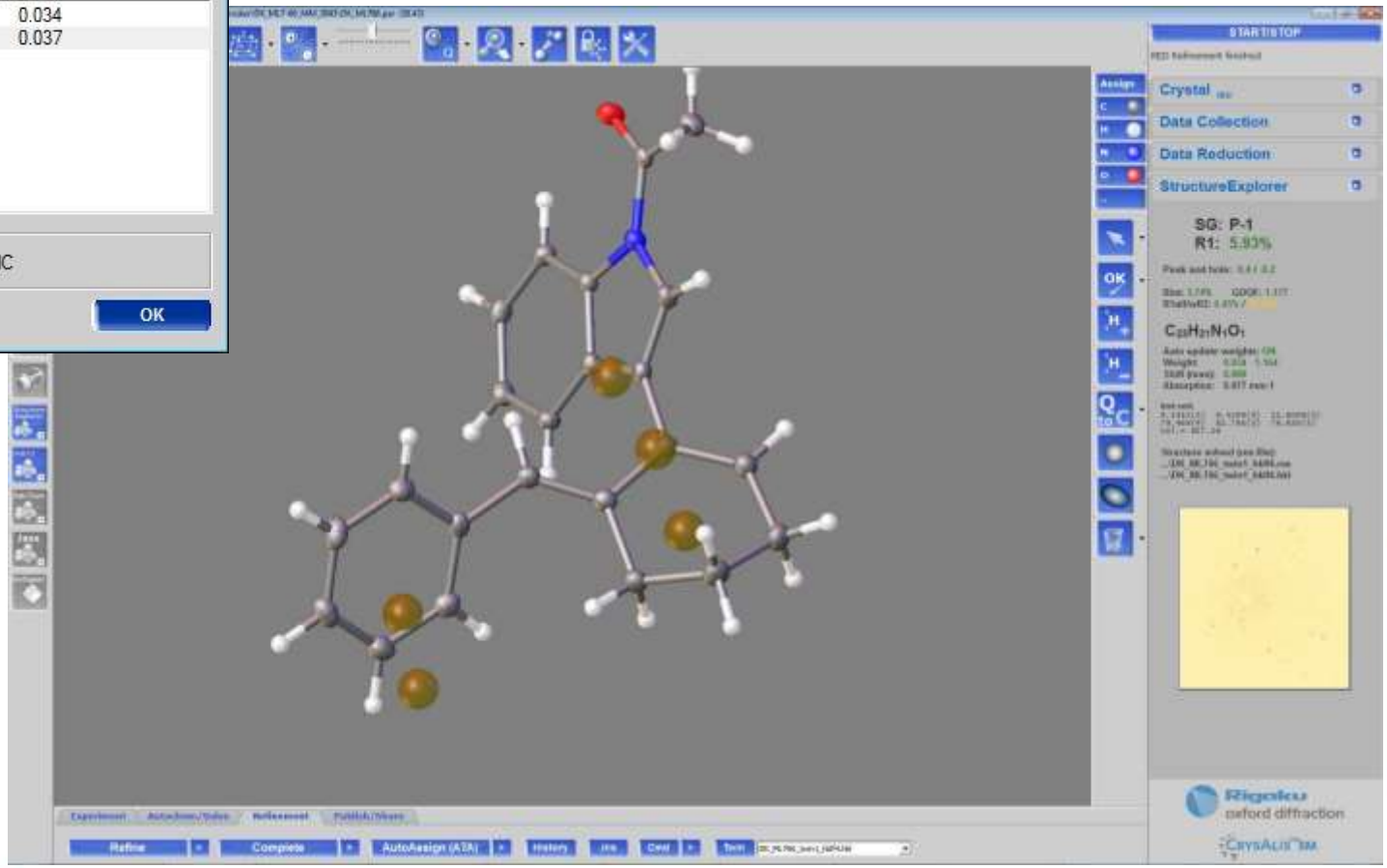
HKLF4 result





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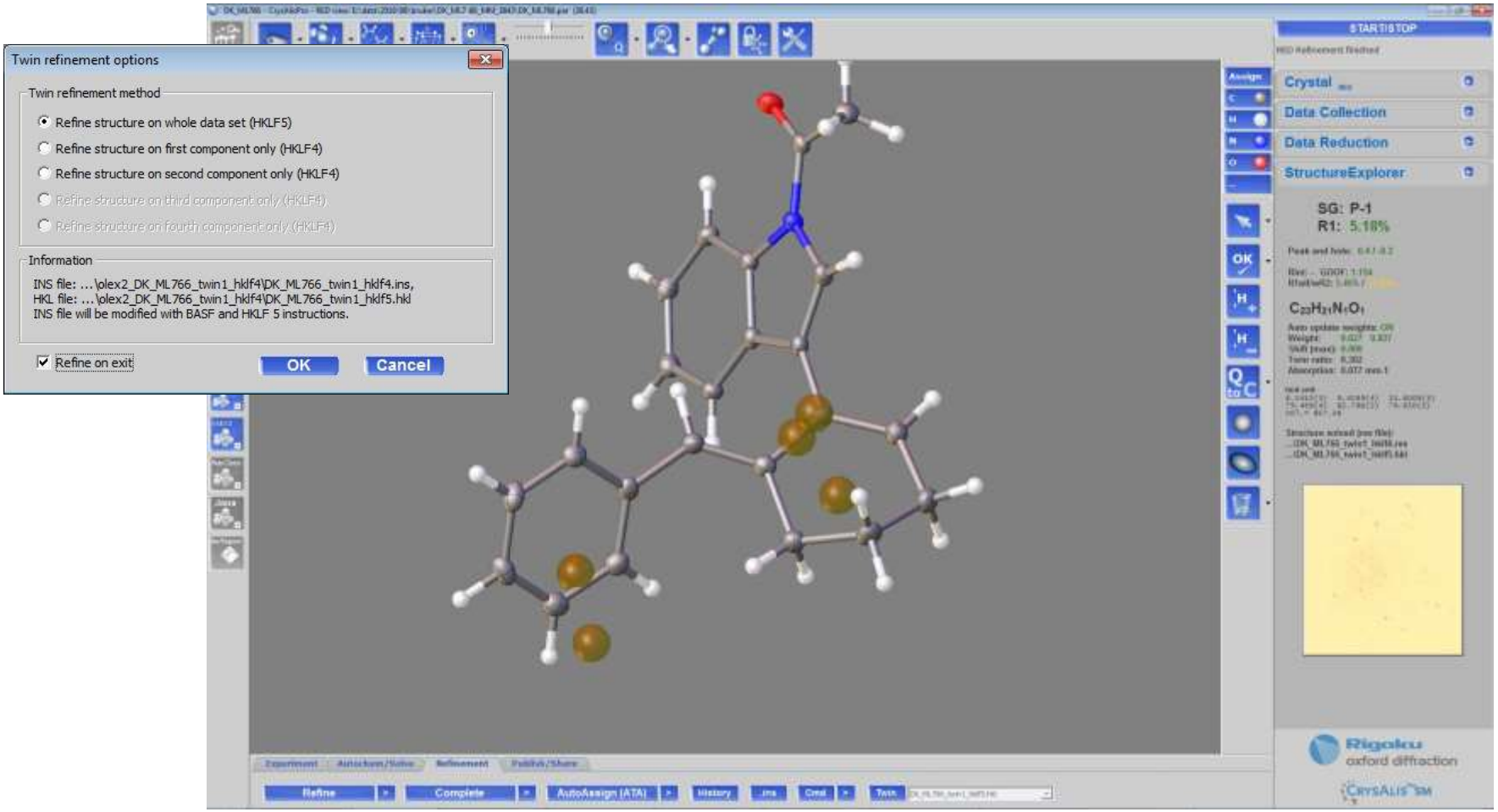
HKLF5 result



Generic image format ‘Esperanto’ generator

- Use of Esperanto format for unknown image formats with no compression or known formats with strange instrument configs
- Esperanto fully supports 4 circle instruments.
- Command ‘dc rit’ rit = raw image transform.
- But it also supports the known formats to handle ‘unusual’, obstinate images.
- Pixel detectors have an automatic dead zone detection based on the special value -1.
- The Esperanto generator uses a proprietary Agilent bit field format. To get back the uncompressed Esperanto version, please use the export function.

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Esperanto with bit field compression and pixel detector support

- For our Esperanto importer we now can use Agilent bitfield compression for Esperanto files. The format is not documented yet.
- There was also a pixel detector flag added to support the implemented pixel detector corrections (`[dsithicknessmmforpixeldetector] - thickness of Si for pixel detectors; the presence of this number signals a pixel detector. Pixel detector gap zones are marked with -1`).
- Publication describes the Esperanto format

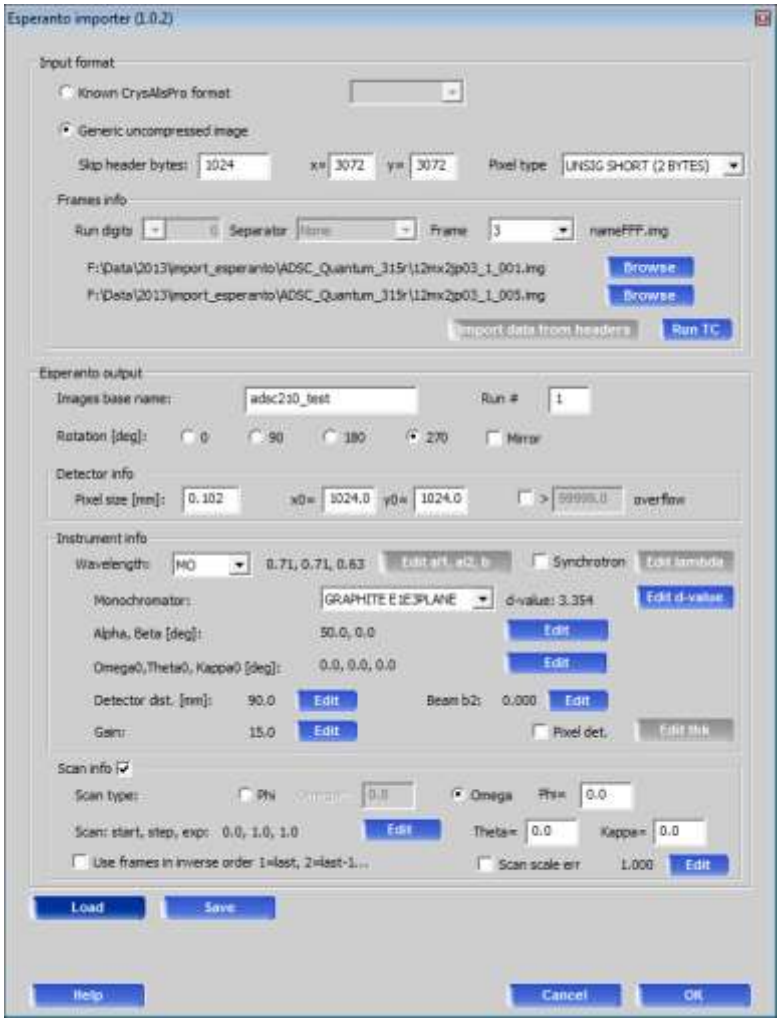
Single-crystal diffraction at the Extreme Conditions beamline P02.2: procedure for collecting and analyzing high-pressure single-crystal data

André Rothkirch, G. Diego Gatta, Mathias Meyer, Sébastien Merkel, Marco Merlini and Hanns-Peter Liermann

J. Synchrotron Rad. (2013). **20**, 711–720

Rigaku oxford diffraction

Dc rit: ADSC 315



- Command dc rit
- Header bytes 1024, x 3072 y 3072 and other info from text header (f.ex with total commander)
- Then esperanto createrunlist
- Slight play in EwaldPro to get the center right.

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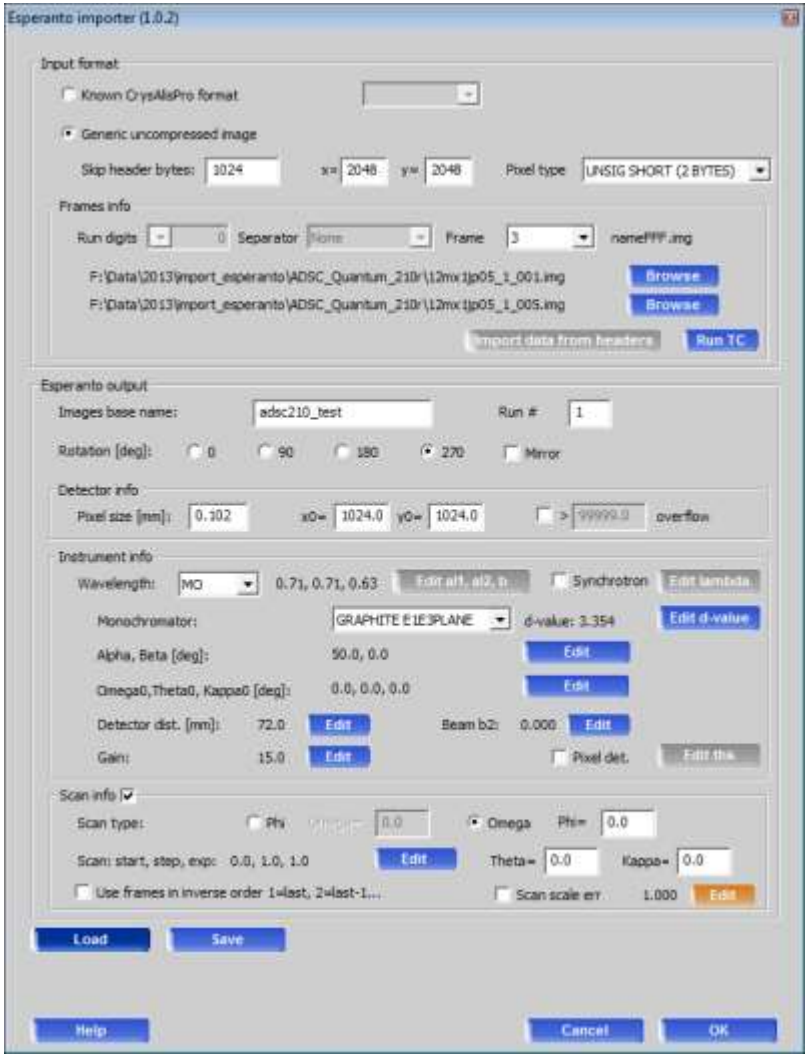
Dc rit: ADSC 210



- Command dc rit
- Header bytes 1024, x 2048 y 20482 and other info from text header (f.ex with total commander)
- Then esperanto createrunlist
- Slight play in EwaldPro to get the center right.

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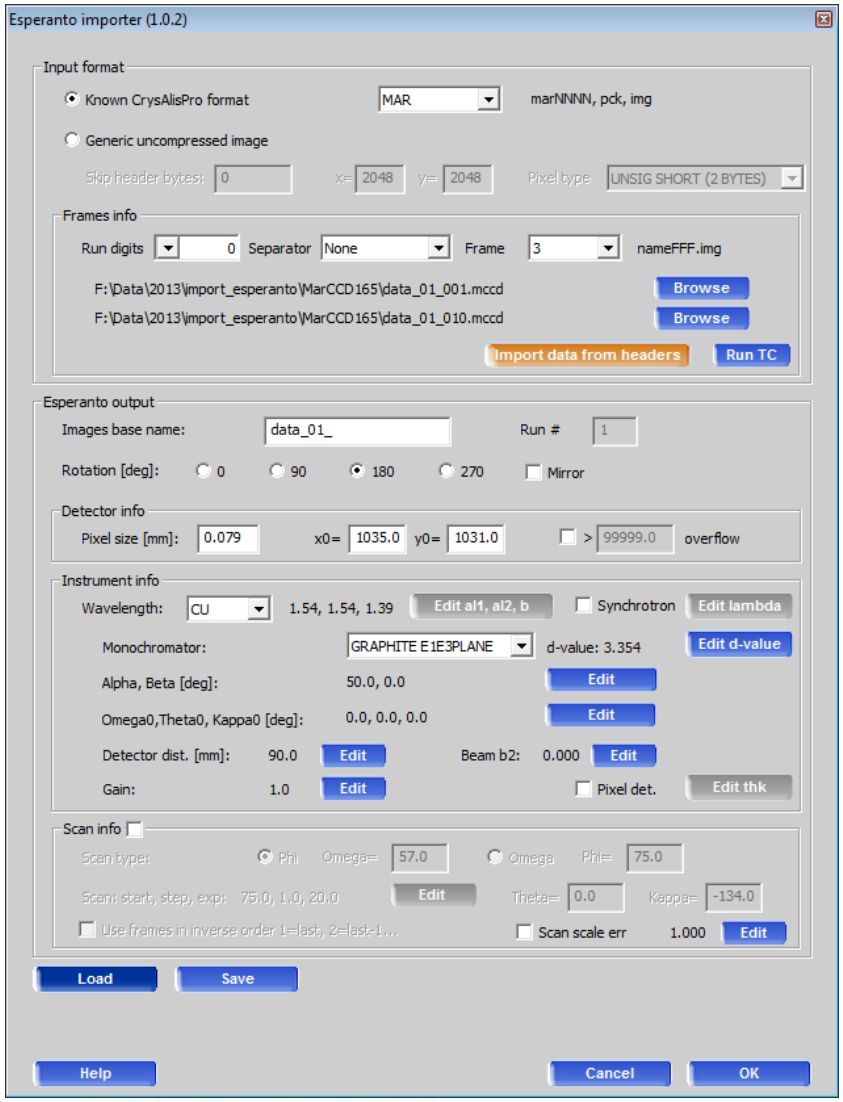
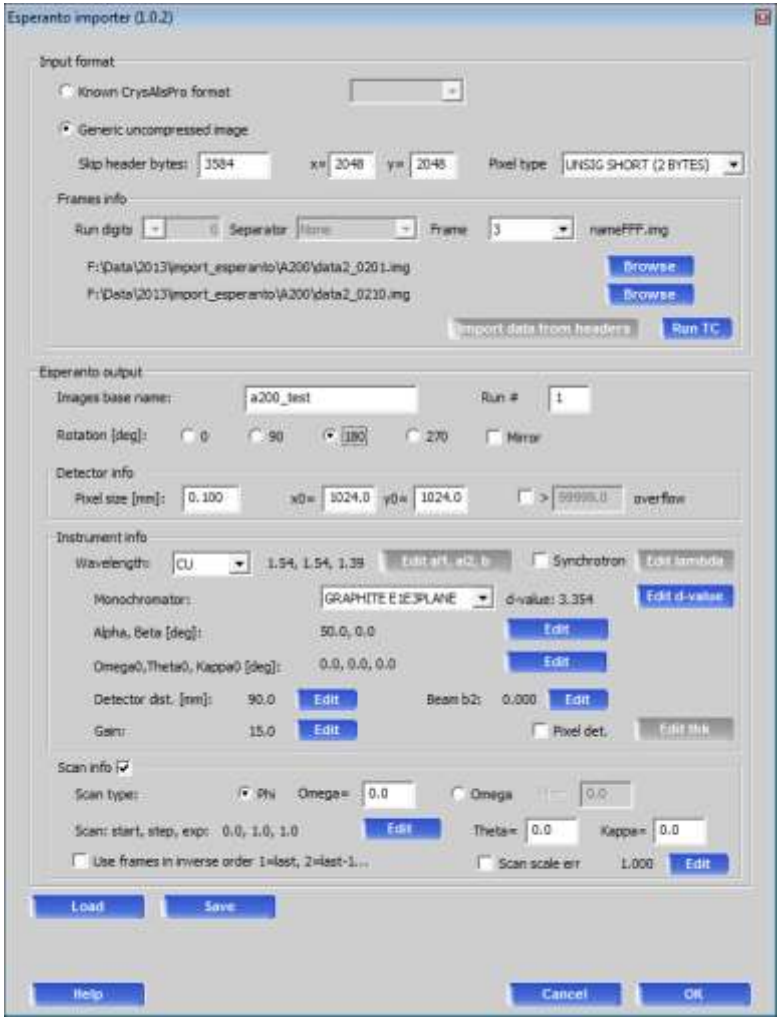
Dc rit: MAR165ccd



- Command dc rit
- Known format MAR (mccd)
- Then esperanto createrunlist
- Slight play in EwaldPro to get the center right.

Rigaku oxford diffraction

Dc rit: A200 detector



- Command dc rit
- Header bytes 3584, x 2048 y 20482 and other info from text header (f.ex with total commander)
- Then esperanto createrunlist
- Slight play in EwaldPro to get the center right.

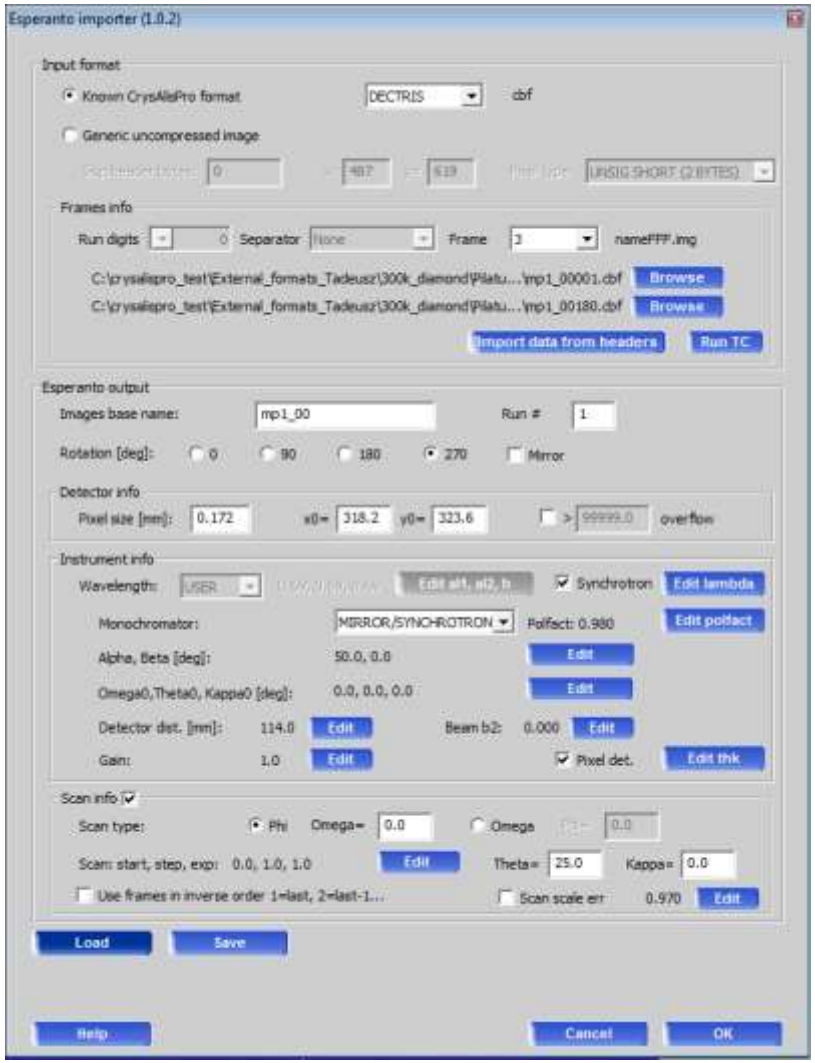
Rigaku
oxford diffraction

Dc rit: Diamond ID 19 Dectris turned

- Command dc rit
- Use of known format dectris. Header values are read.
- Camera turned 270deg. Non-square detector is padded by zeros.
- The header scan values are wrong by 3% (Scan scale err 0.97)
- Then esperanto createrunlist
- Slight play in EwaldPro to get the center right.
- The several cycles to refine instrument model.

Rigaku
oxford diffraction

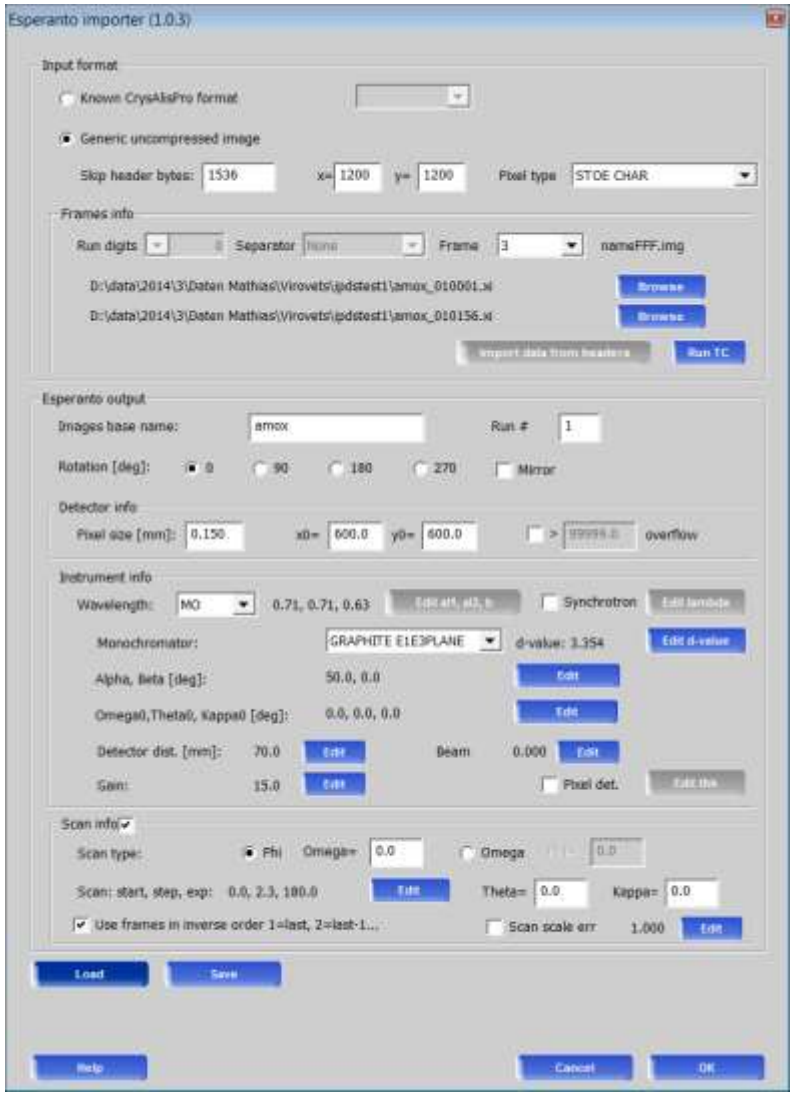
Dc rit: Diamond ID 19 Dectris turned II



- Command dc rit
- Use of known format dectris. Header values are read.
- Camera turned 270deg. Non-square detector is padded by zeros.
- This data had NO scan scale error!
- Then esperanto createrunlist
- Slight play in EwaldPro to get the center right.
- The several cycles to refine instrument model.

Rigaku
oxford diffraction

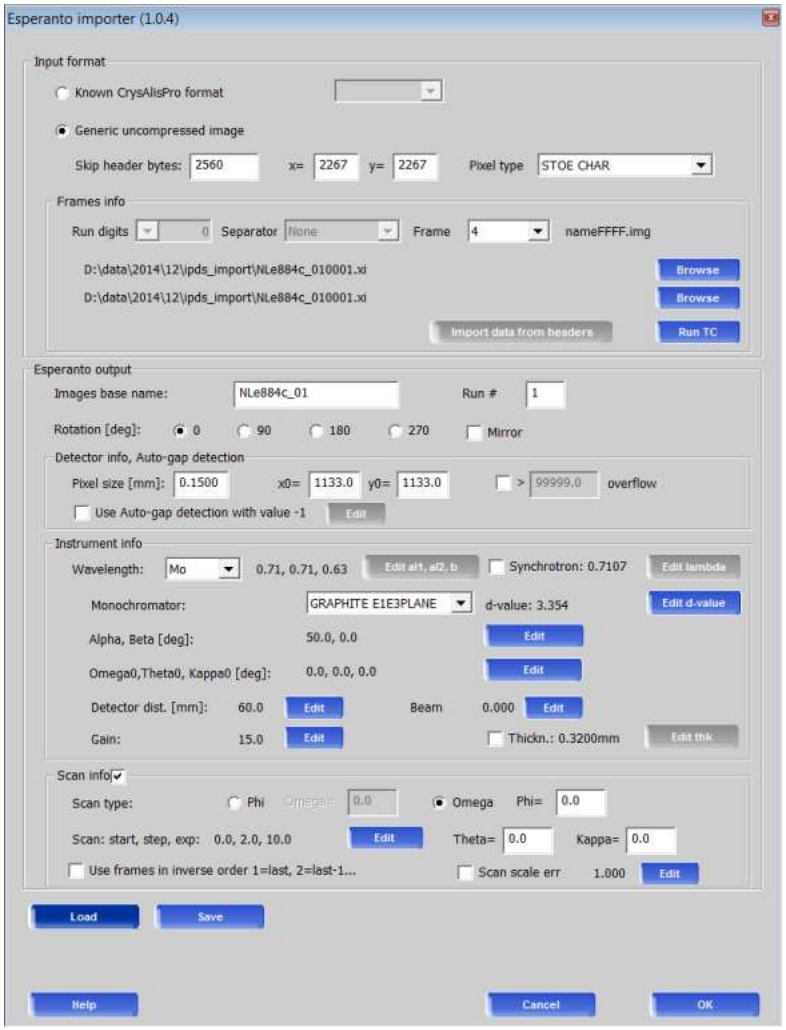
Dc rit: IPDS



- Command dc rit/Import button on power toolbar
- Read detector information from the sum file of IPDS (0.15mm pix, cen x=600, y=600)
- Stoe char as pixel type; .xi files (this is OD compression…)
- Make sure to use resolution limit due to round IP image (Mo typical 0.809Ang)

Rigaku oxford diffraction

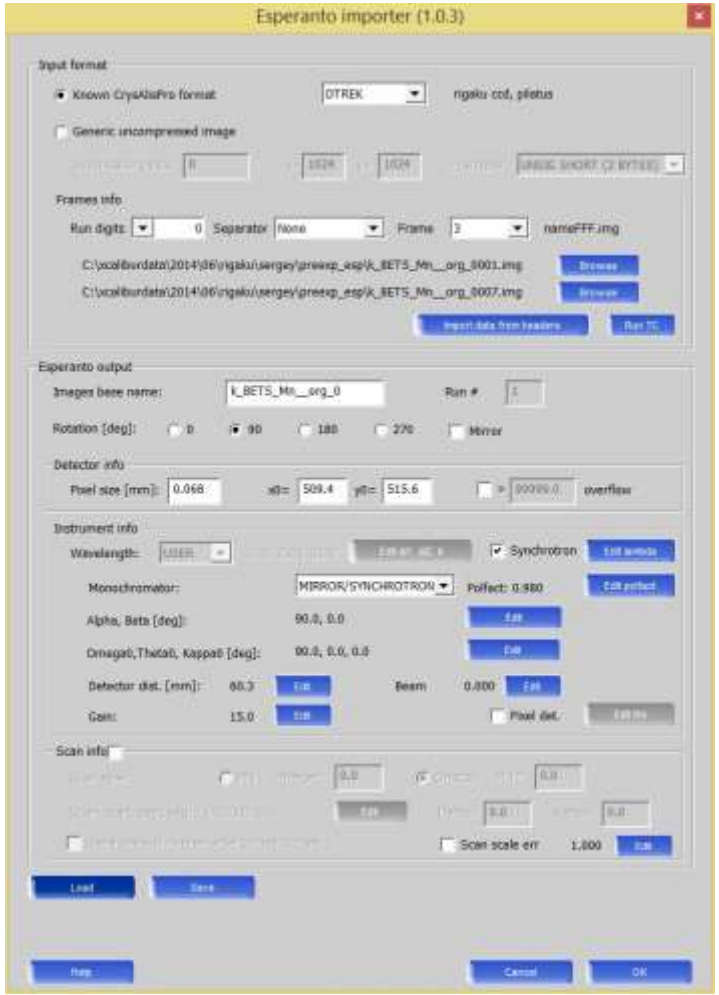
Dc rit: IPDS 2



- Command dc rit/Import button on power toolbar
- Read detector information from the sum file of IPDS (0.15mm pix, cen x=1133, y=1133)
- Stoe char as pixel type; .xi files (this is OD compression…)
- Make sure to use resolution limit due to round IP image (Mo typical 0.809Ang)

Rigaku oxford diffraction

Dc rit: dtrek frame from Japanese synchrotron



- Command dc rit/Import button on power toolbar
- The issue was here that the dtrek image was turn 90deg relative to the inhouse image. The dtrek createrunlist would not work on this.
- Thus the ‘dc rit’ command can be used to handly obstinate known images…

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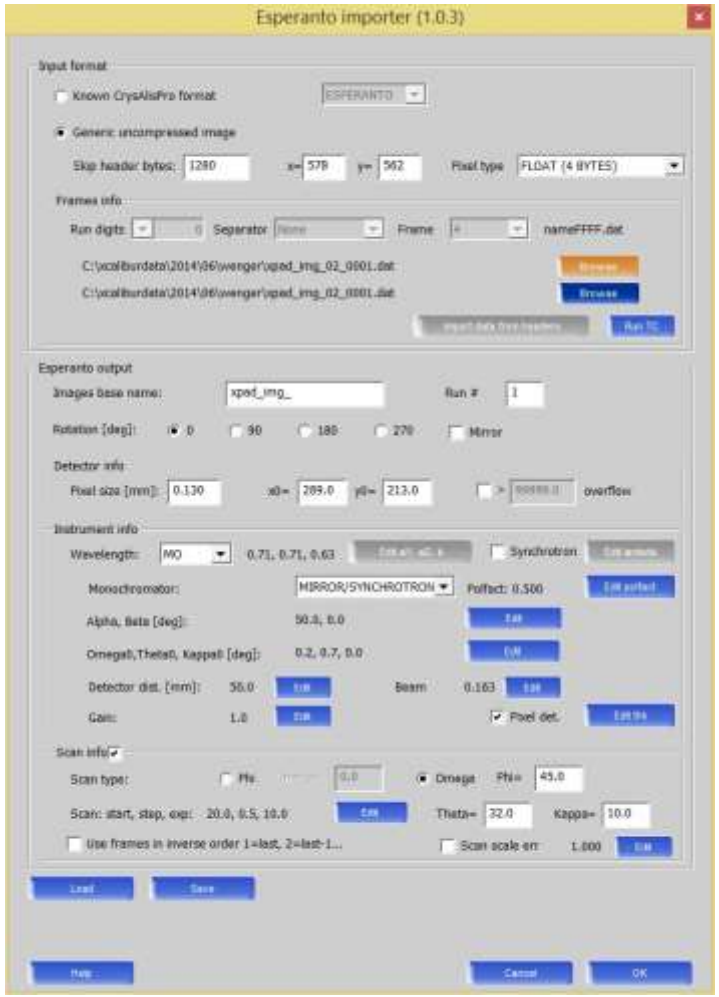
oxford diffraction

Dc rit: xpad detector



- Command dc rit/Import button on power toolbar
- The xpad detector is developed in France
- One of it's raw format can be channelled through the Esperanto importer
- As the header info is unknown, it has to be given in the scan info section.
- Provide the raw data file contains the -1 marker for pixel detectors the esperanto createrunlist command will automatically create a ccd file with dead zones.
- Such formats have to be transformed run by run as there is only one field for scan info.

Rigaku
oxford diffraction

Data finalization – optimal data

- Problems with…

- Experiment
- Unit cell
- Data reduction
- Finalization
- Pseudo symmetry, twinning, incommensurate

Experiment

- Problems with…

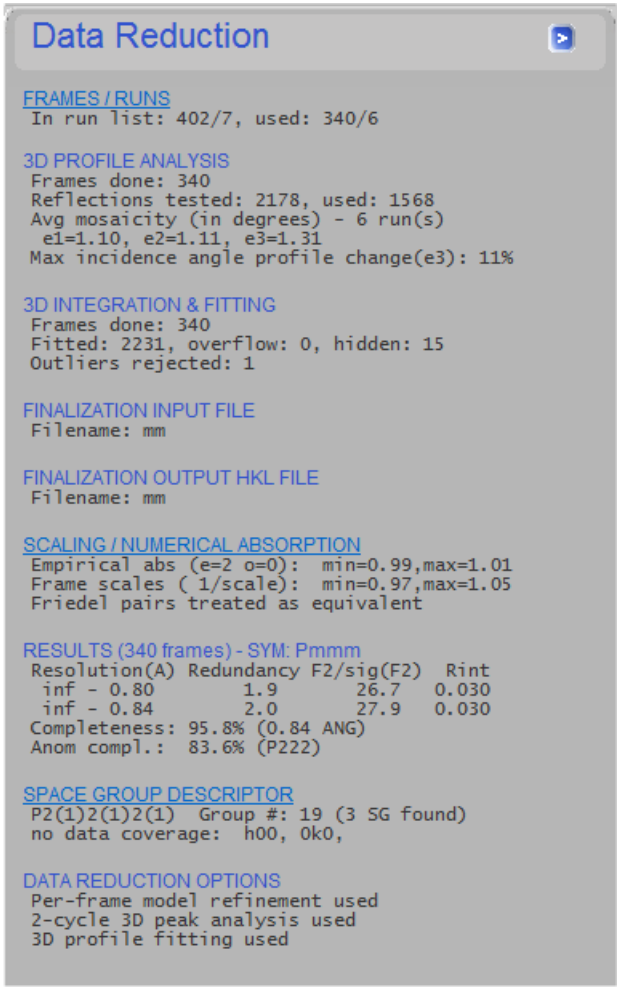
- Exposure time too low – diffraction limit
- De-ice
- Movie missing
- Centering – sample mount
- Choice of wavelength

Approach a data set…

- Inspect executive tab

- Warning signs:

- Run list incomplete
- High mosaicity
- Scaling unusual
- I/sig low; low redundancy
- SG issues



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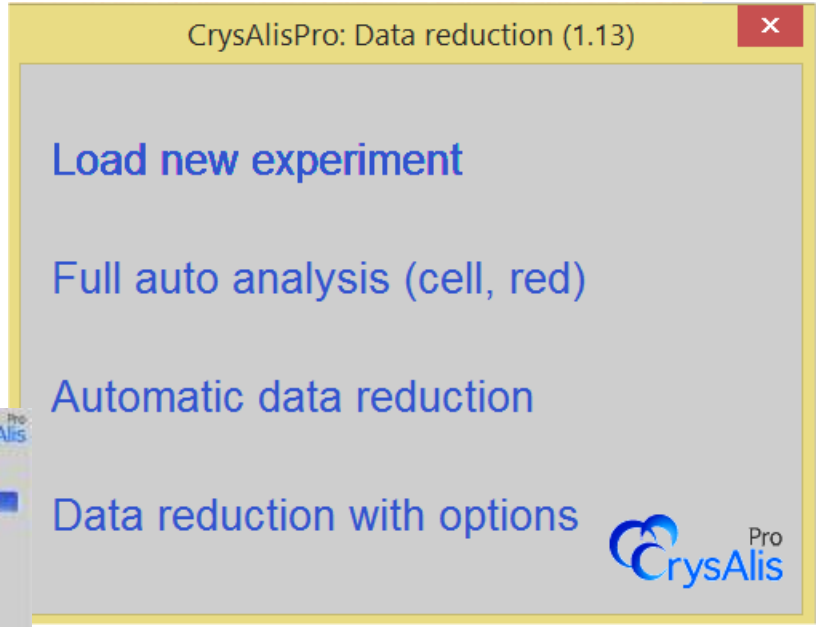
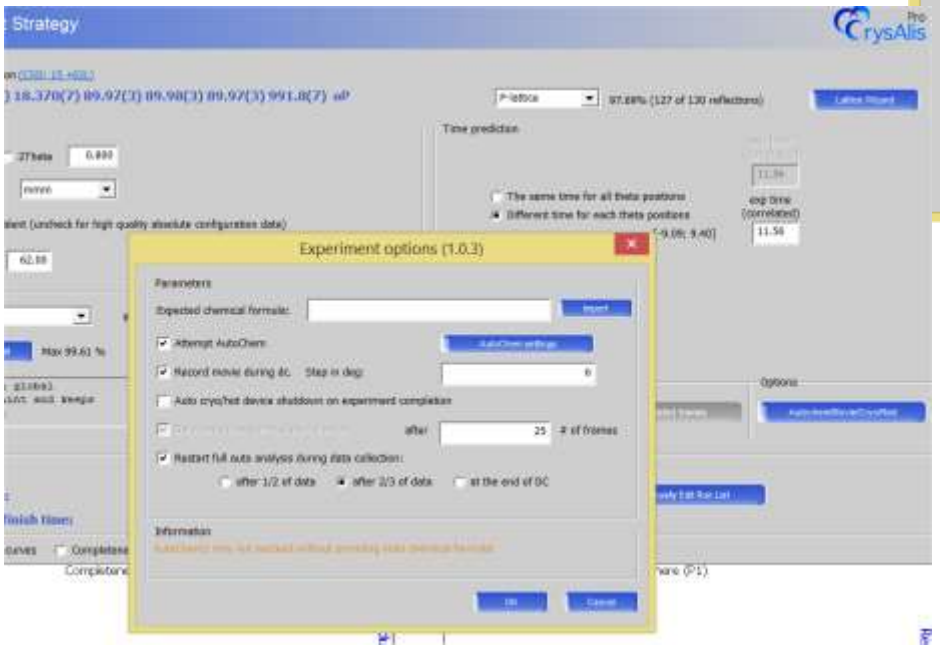
Approach a data set…

- Run ‘Full auto analysis’ on all data
- Concurrent may get stuck





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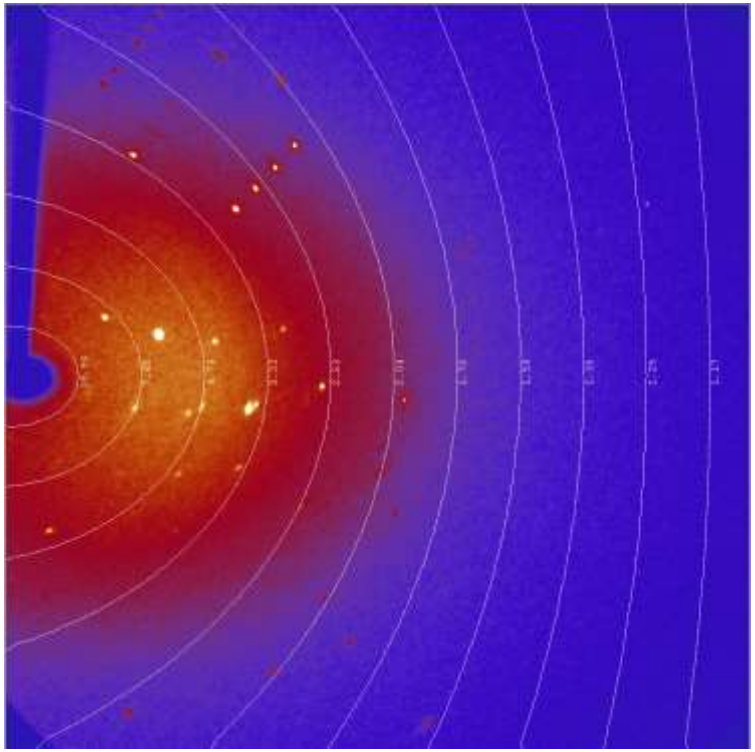
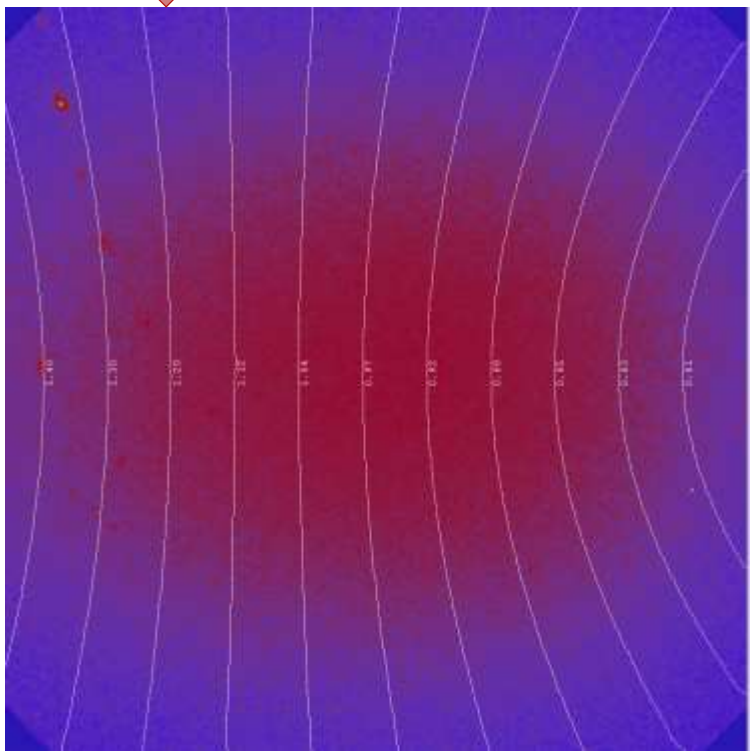
Approach a data set…

- Inspect frames
  - No diffraction at high angle → cut the data to that resolution

Diffraction limit!





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Approach a data set…

- Inspect frames:

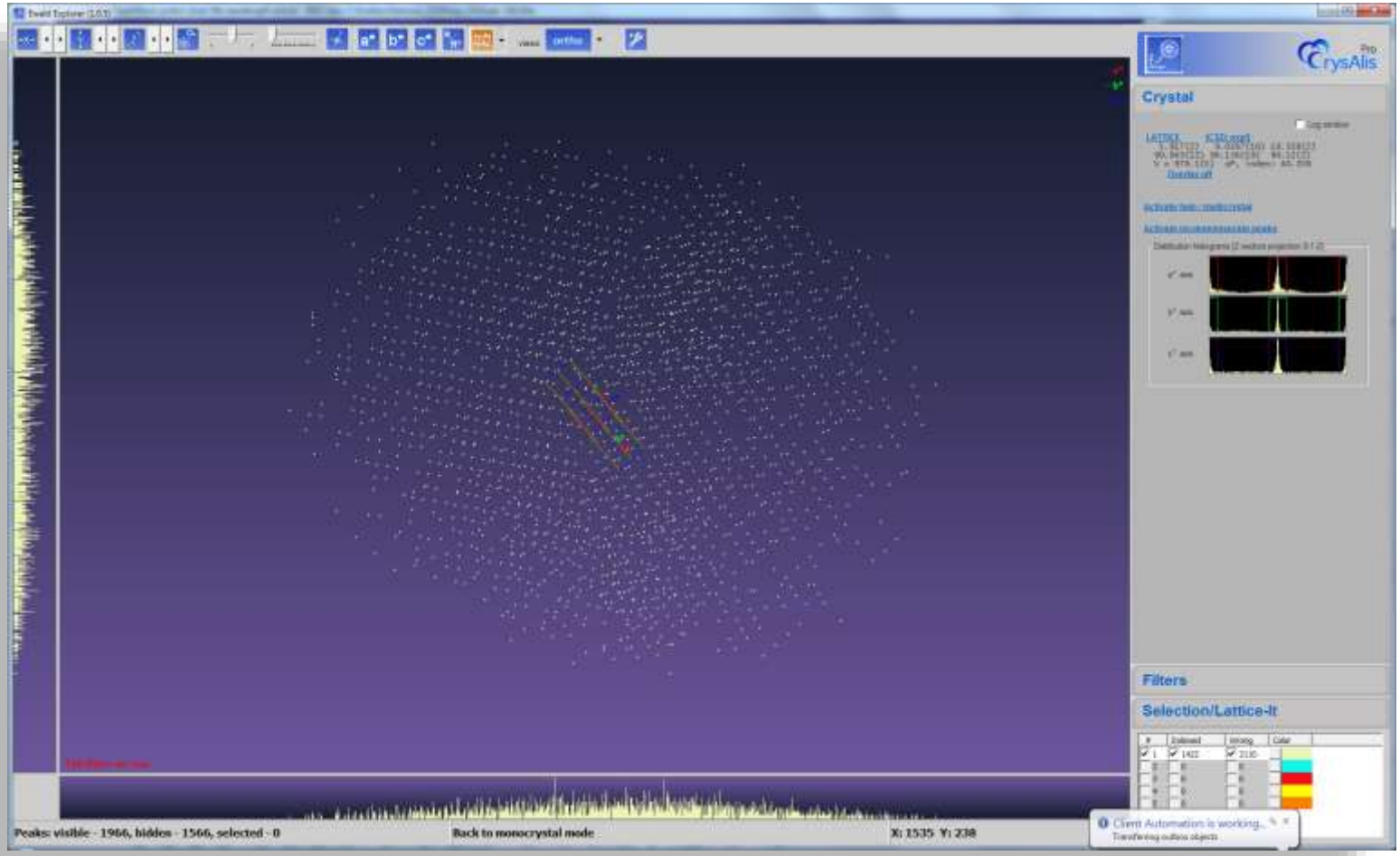
- Low/high background
- Diffuse scattering, split reflections, twin
- Empty frames, strange frames

- Inspect the sample movie (if you have it…):

- Sample mounting

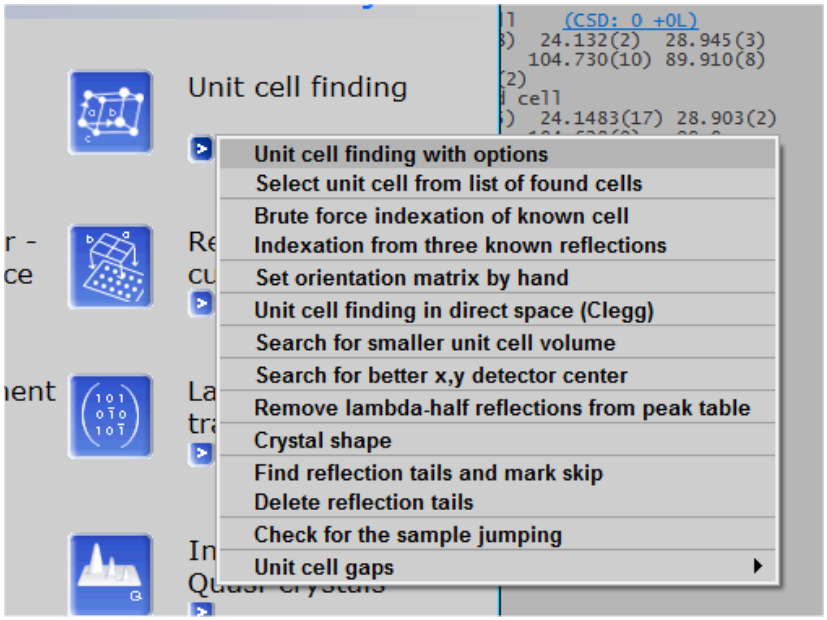
Unit cell…

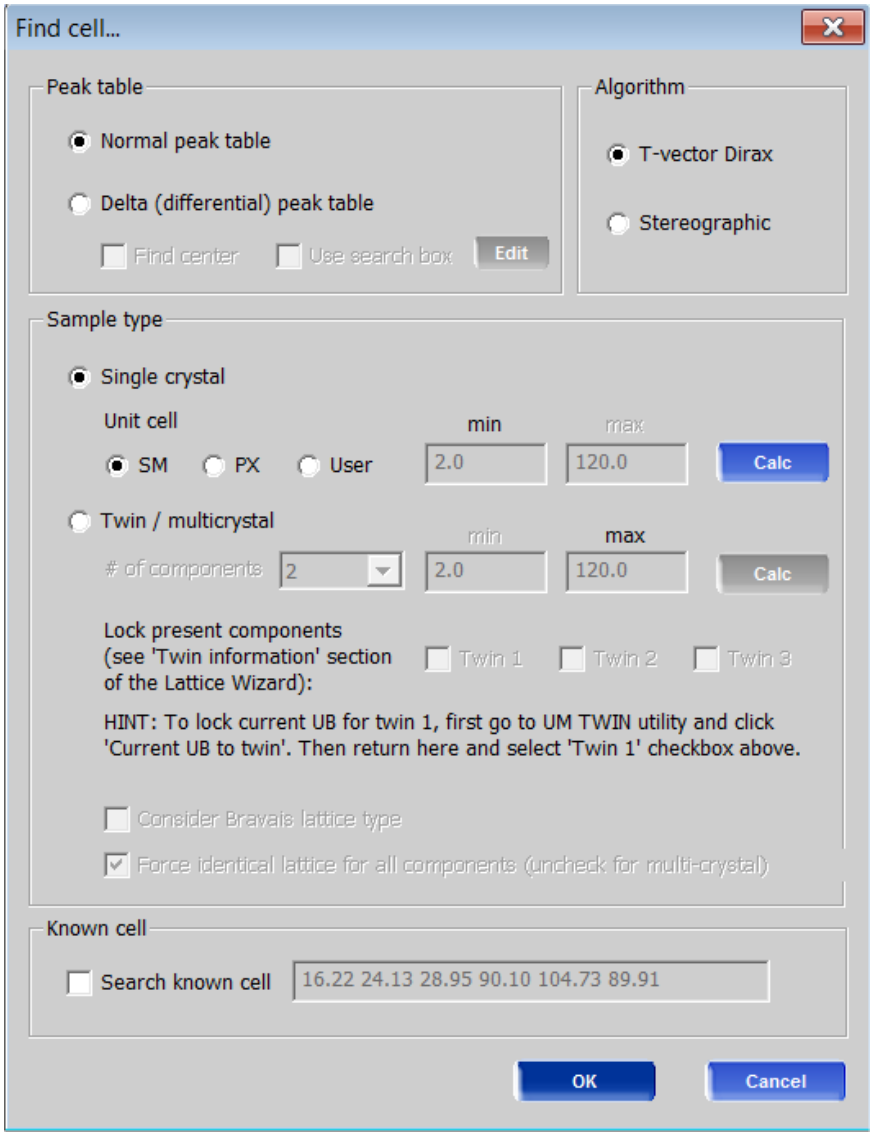
- Ewald Explorer



Rigaku
oxford diffraction

Unit cell finding – Automatic unit cell finding





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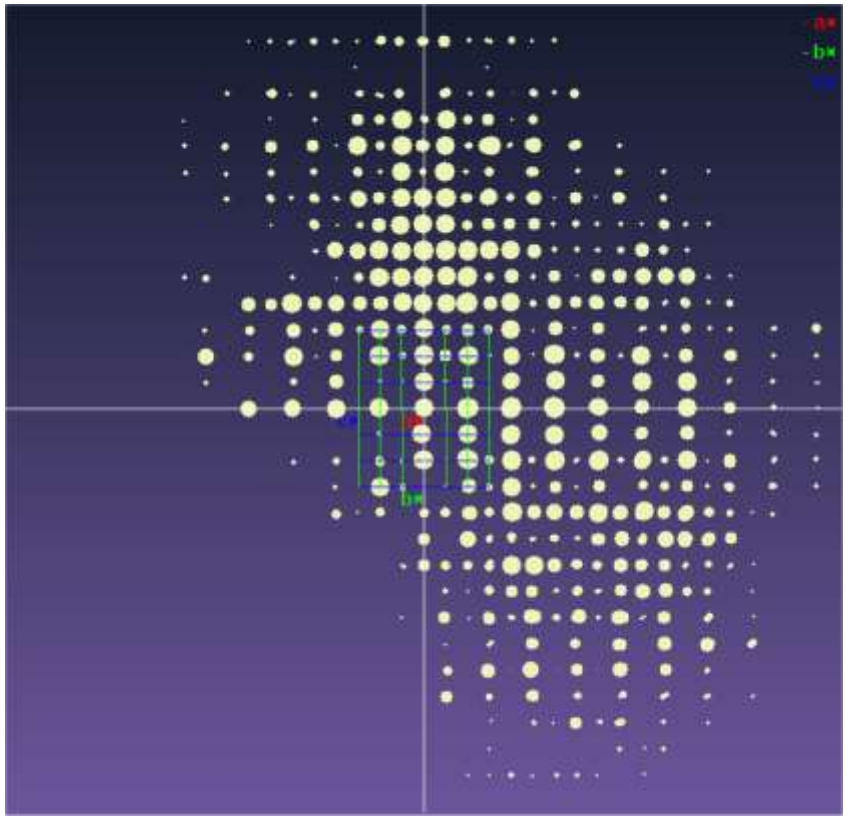
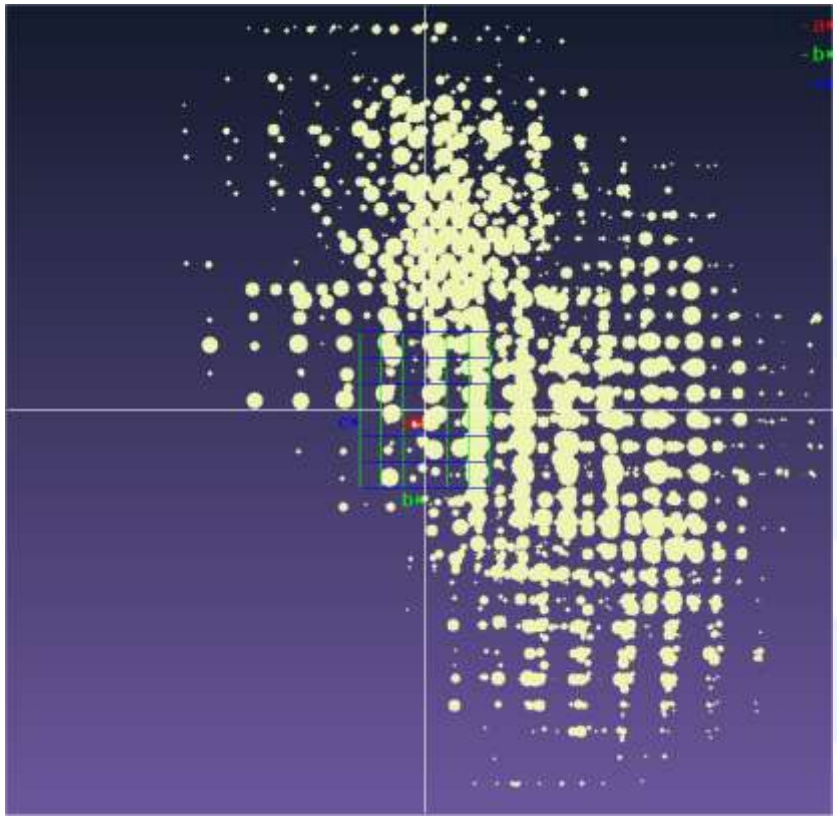
Unit cell finding –
Influence of bad instrument model



Good instrument model



Bad instrument model:

Beam center deviation 40 pix

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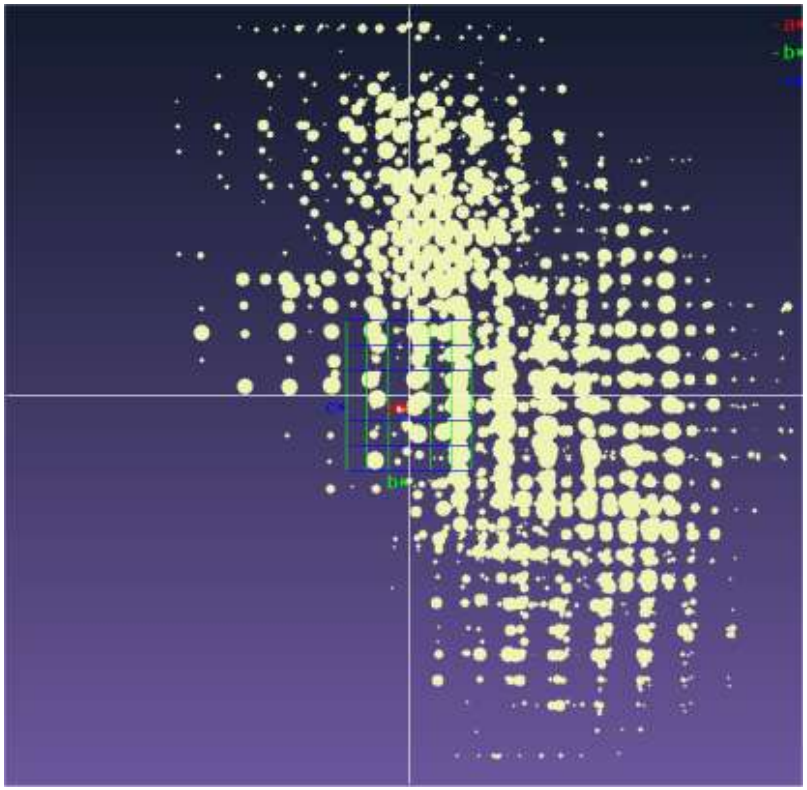
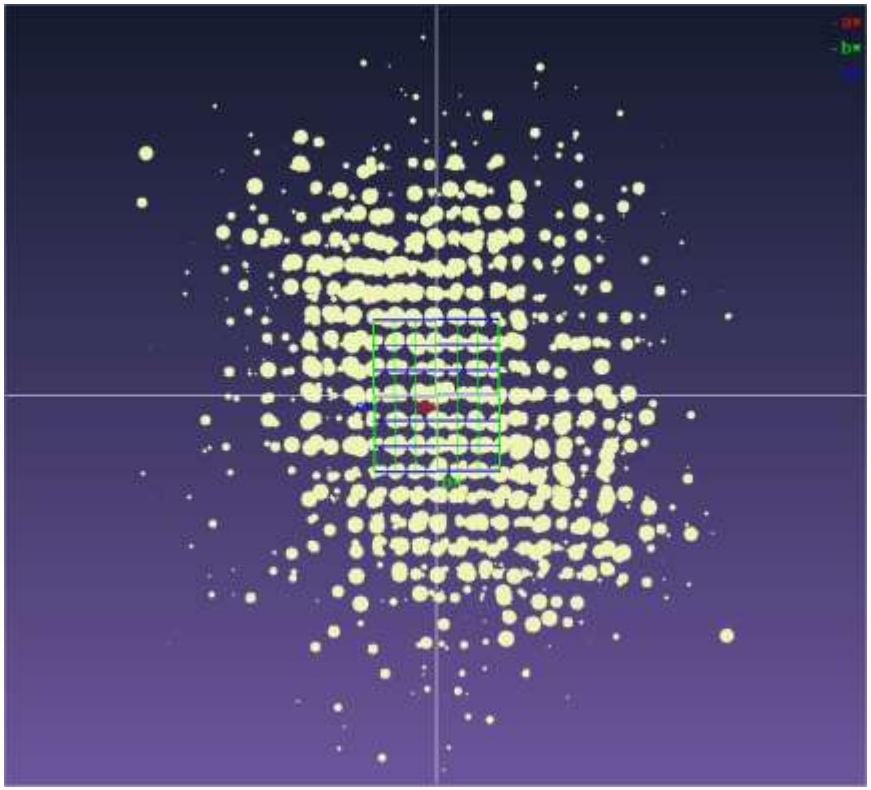
Unit cell finding –
Influence of bad instrument model



Bad instrument model:

Beam center deviation 40 pix



Bad instrument model:

Delta-peak table

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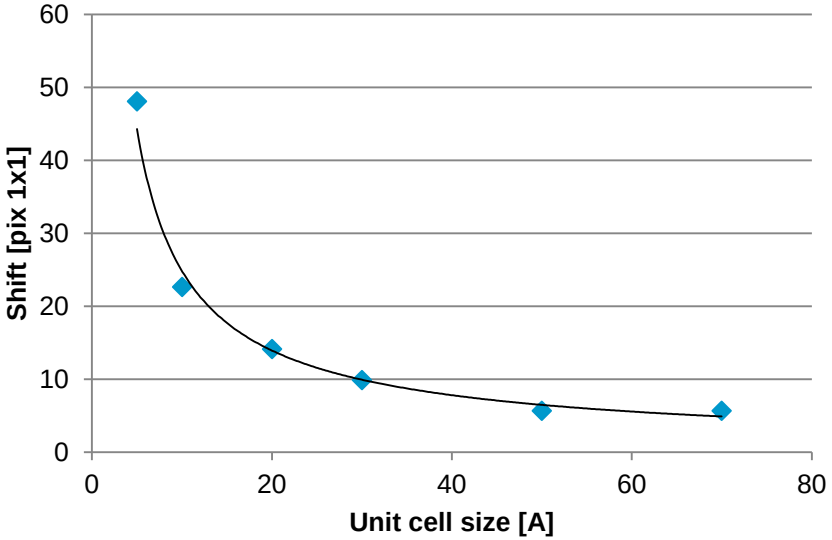
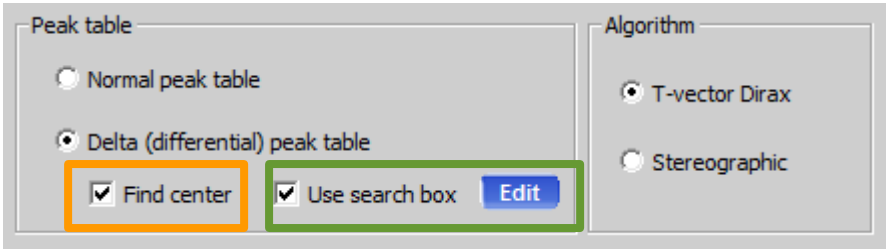
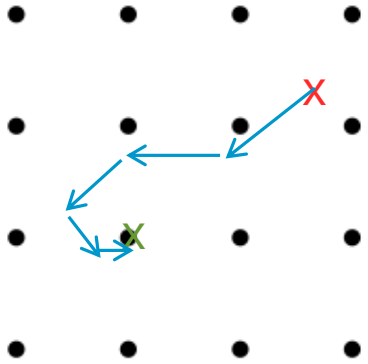
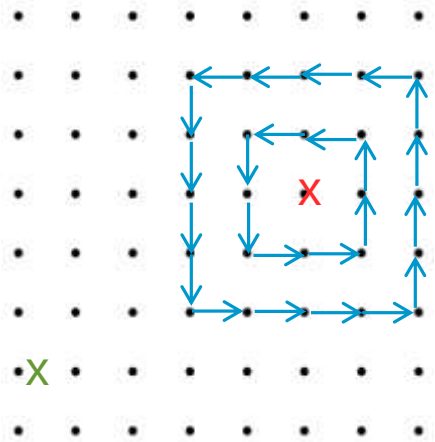
Unit cell finding –
Influence of bad instrument model



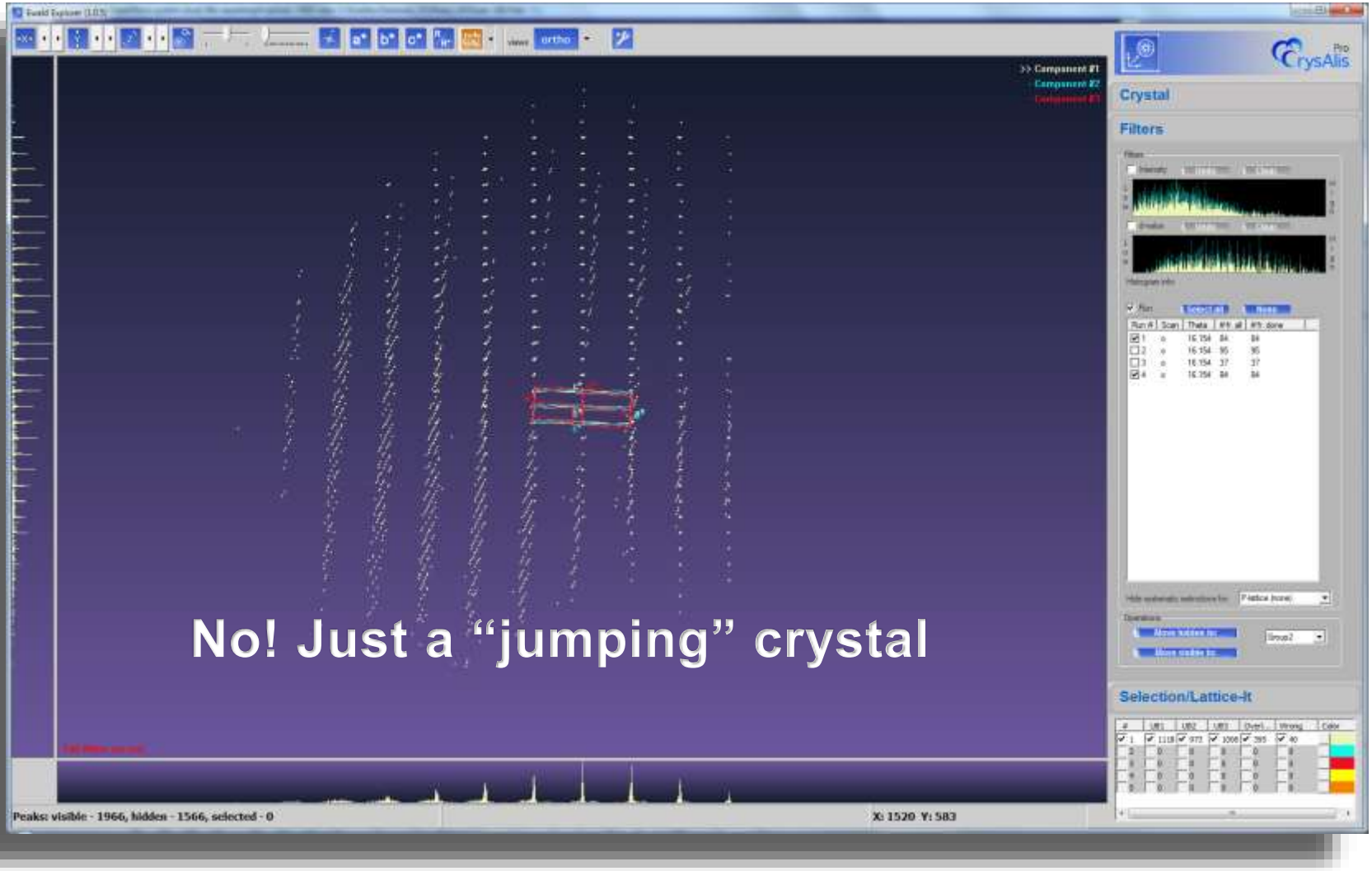






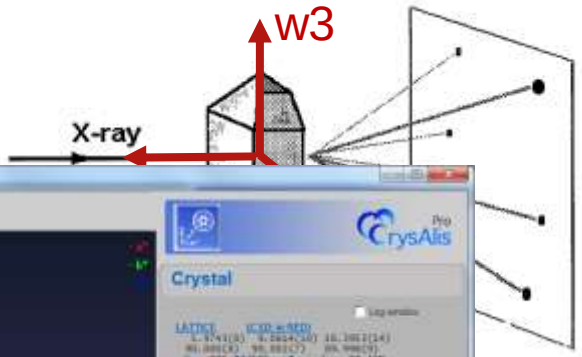
Rigaku
oxford diffraction

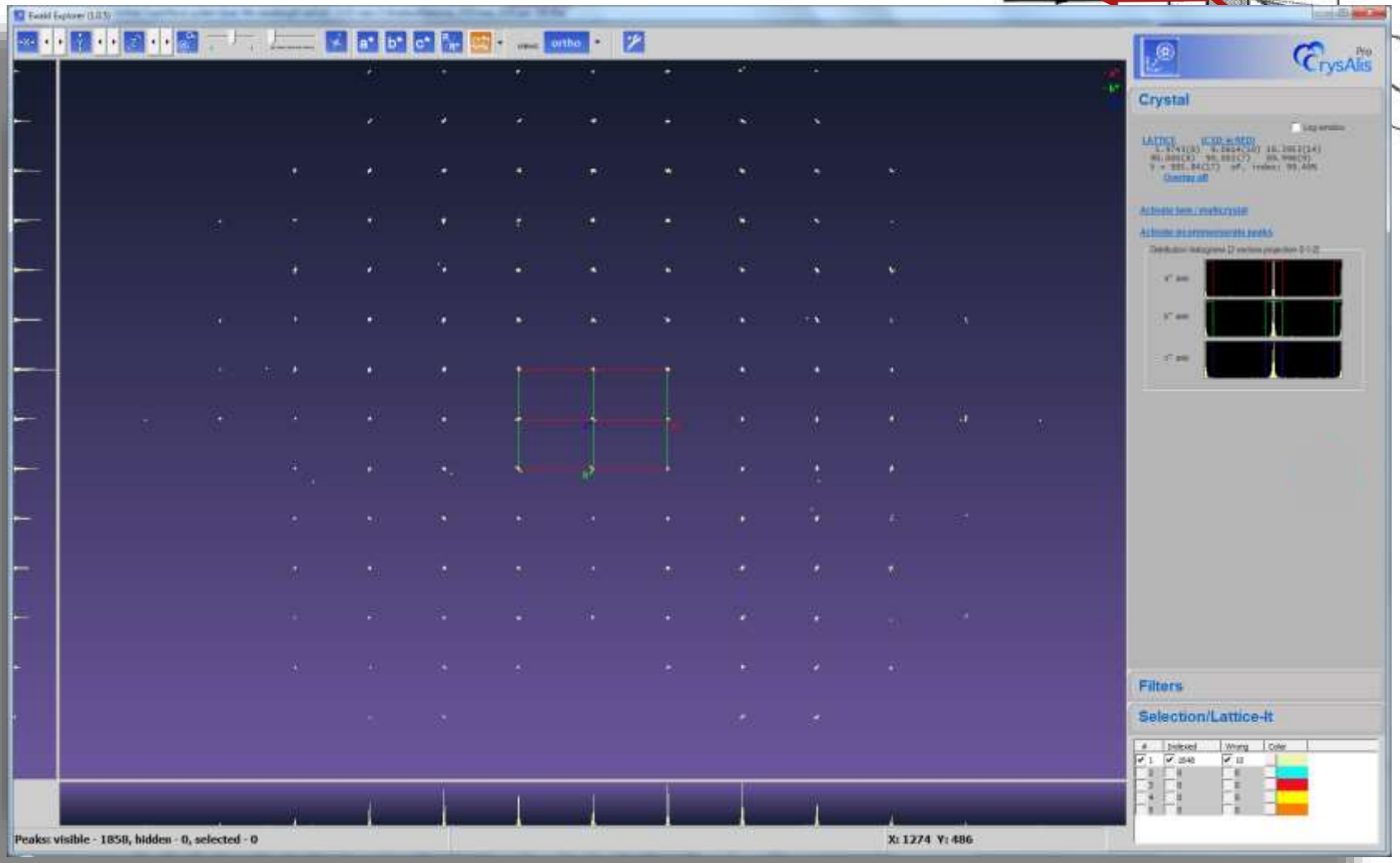
Unit cell (twin vs. Jump)…



Rigaku
oxford diffraction

Unit cell (wobble).





Rigaku
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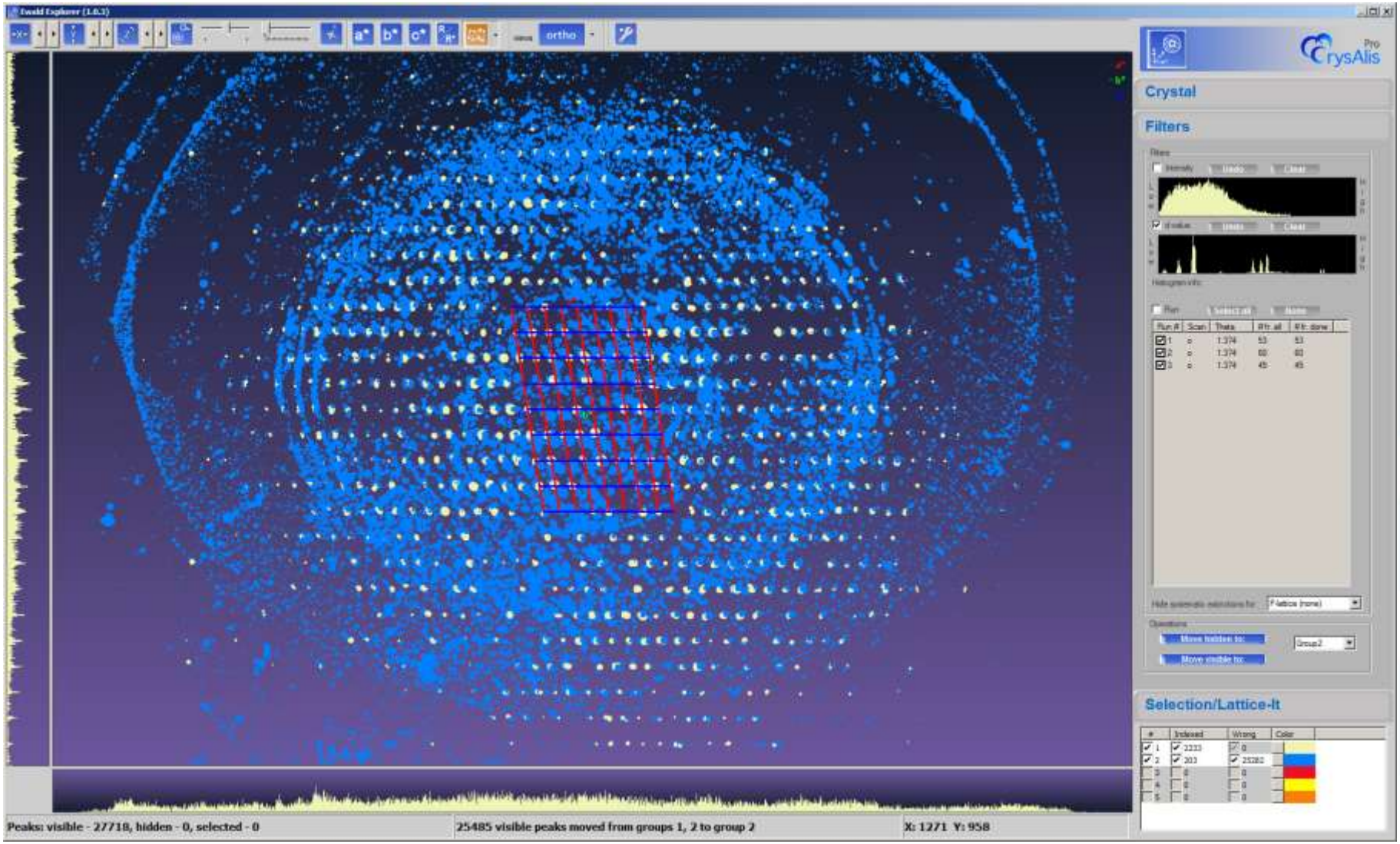
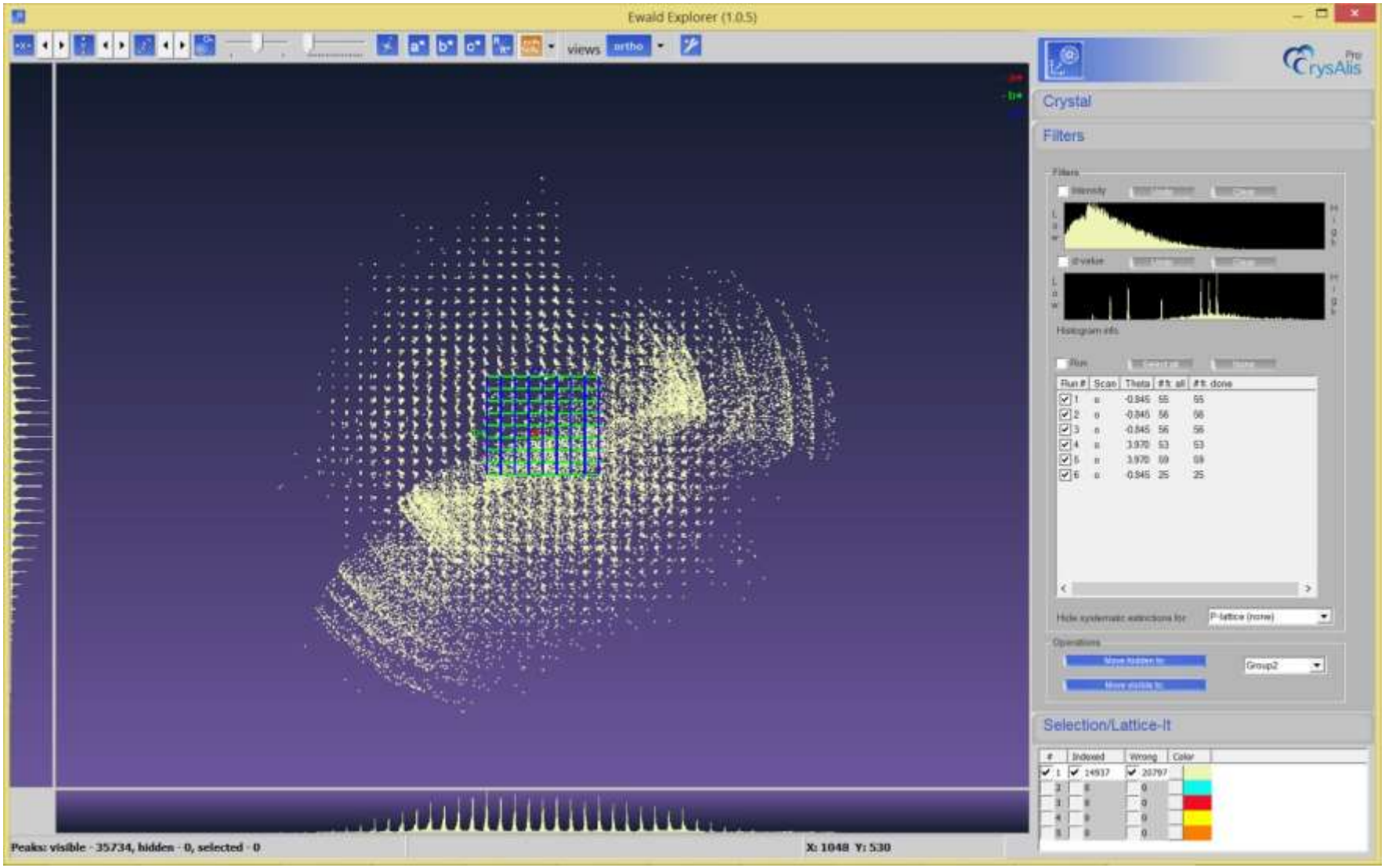
Unit cell (ice ring)…



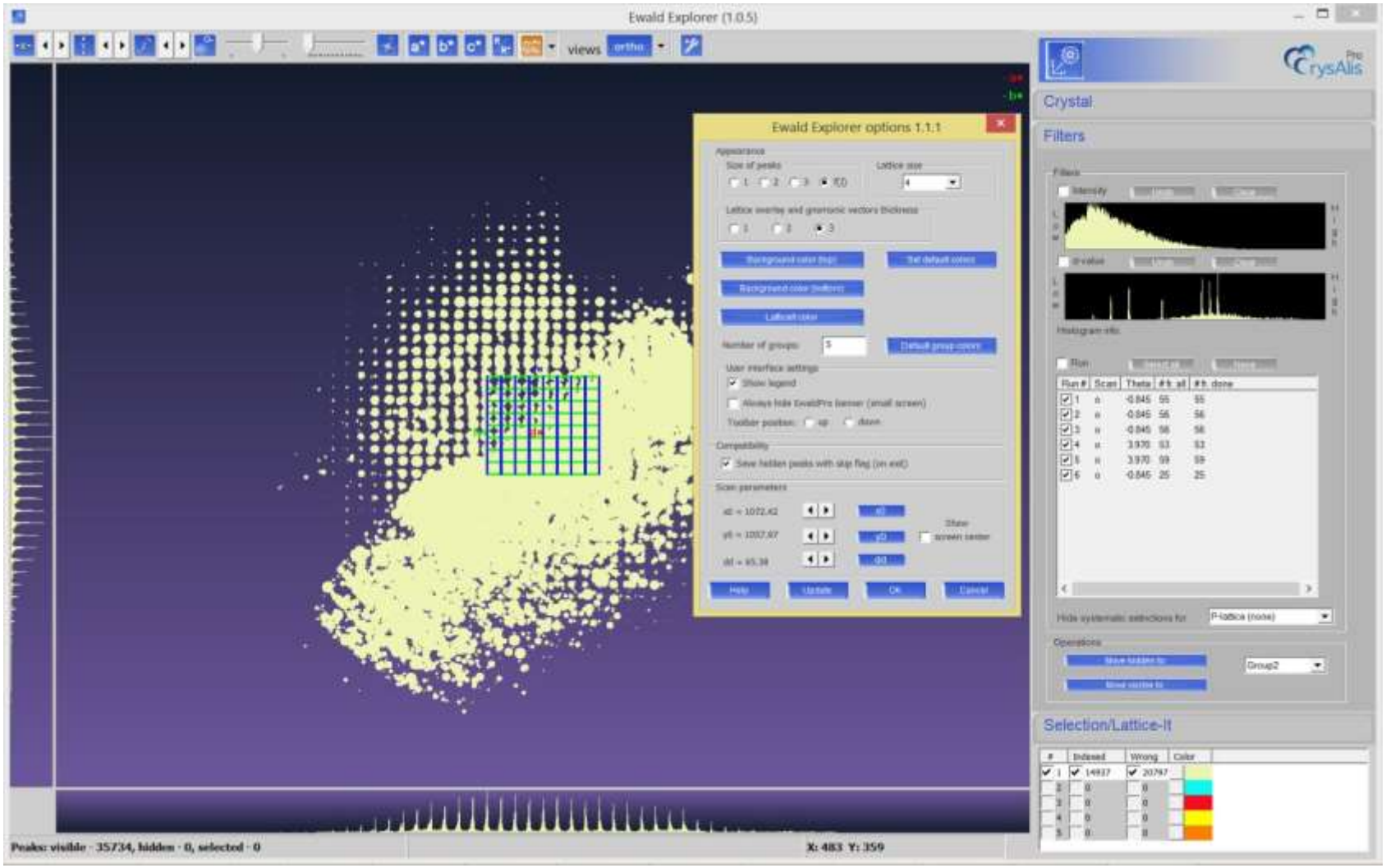
Rigaku
oxford diffraction

Unit cell (filters)…



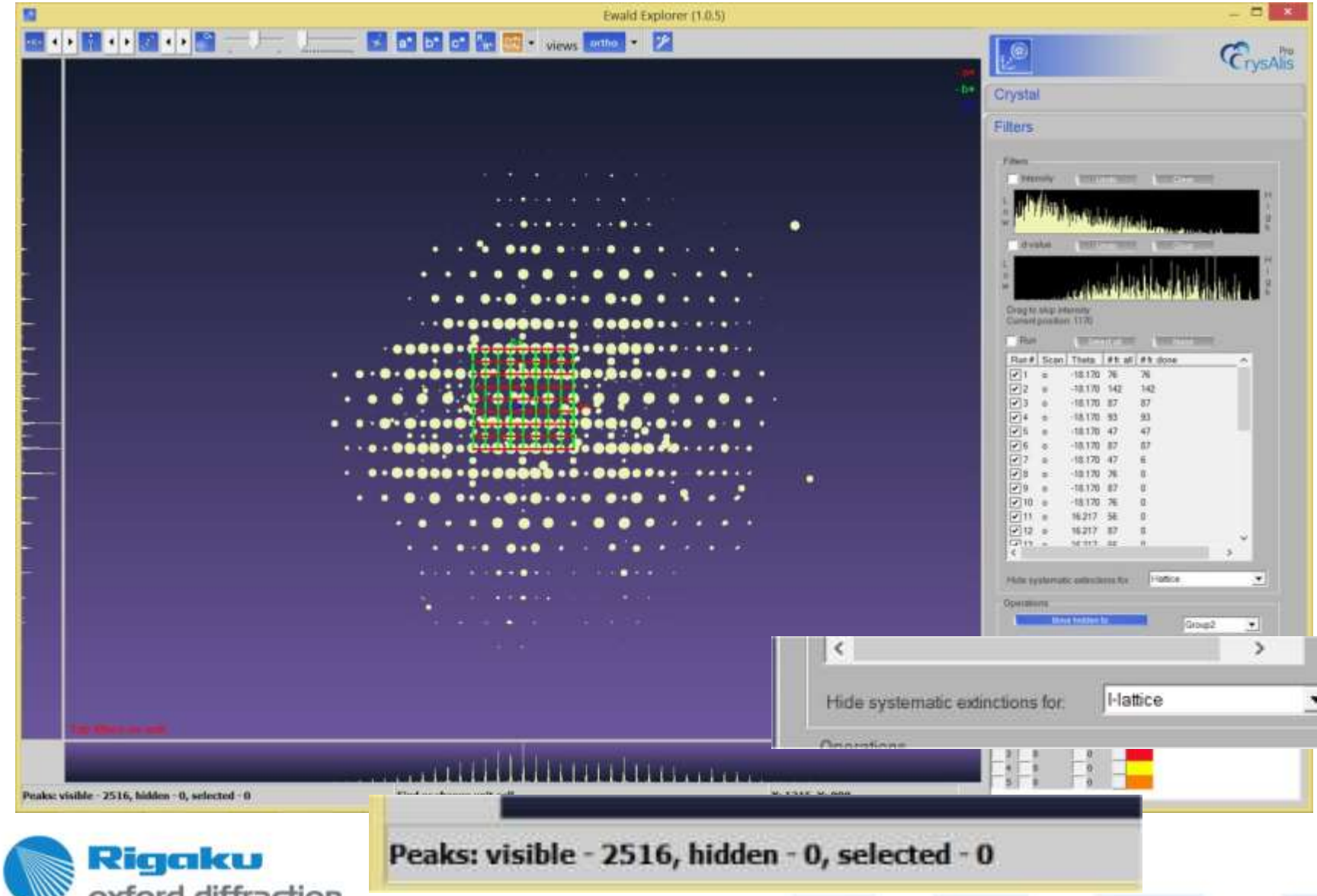
Rigaku
oxford diffraction

Unit cell (filters)…



Rigaku
oxford diffraction

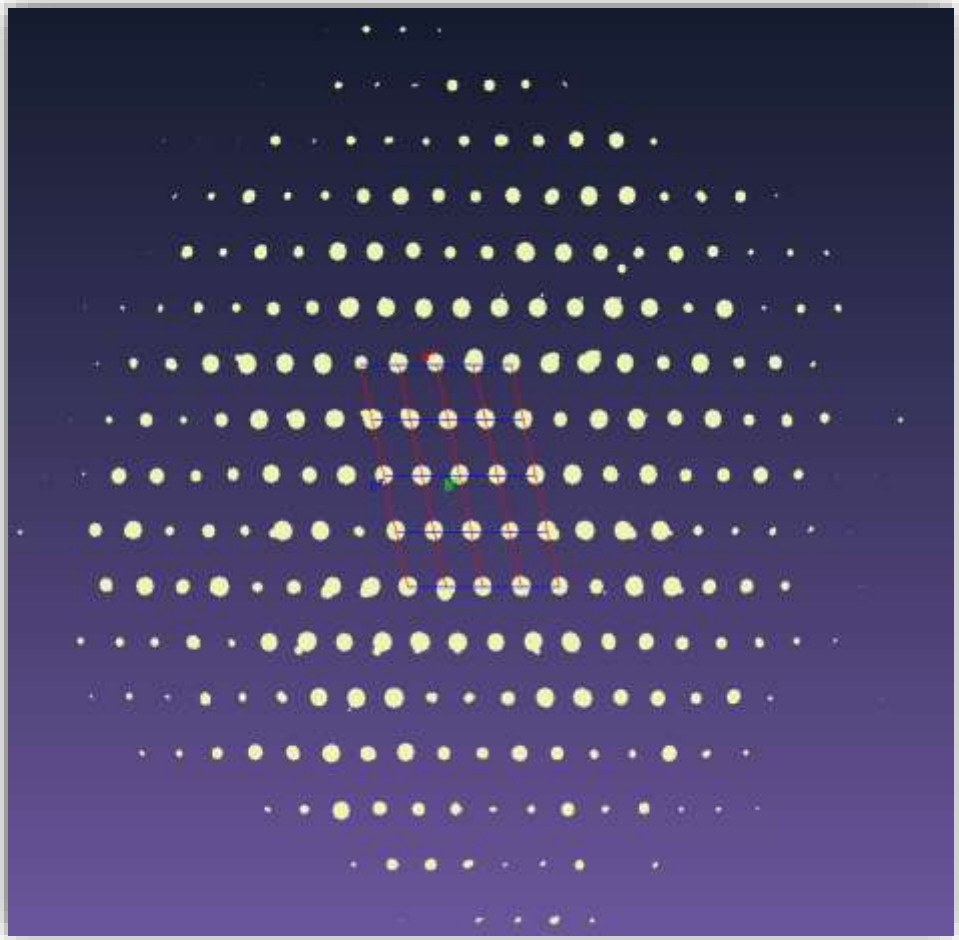
Unit cell (filters)…



Rigaku
oxford diffraction

Ewald^{Pro} Collapse view

Collapse peak view – construction



1. Lattice vectors are multiplied by lattice overlay size
2. Subtract lattice vectors until given peak hits range

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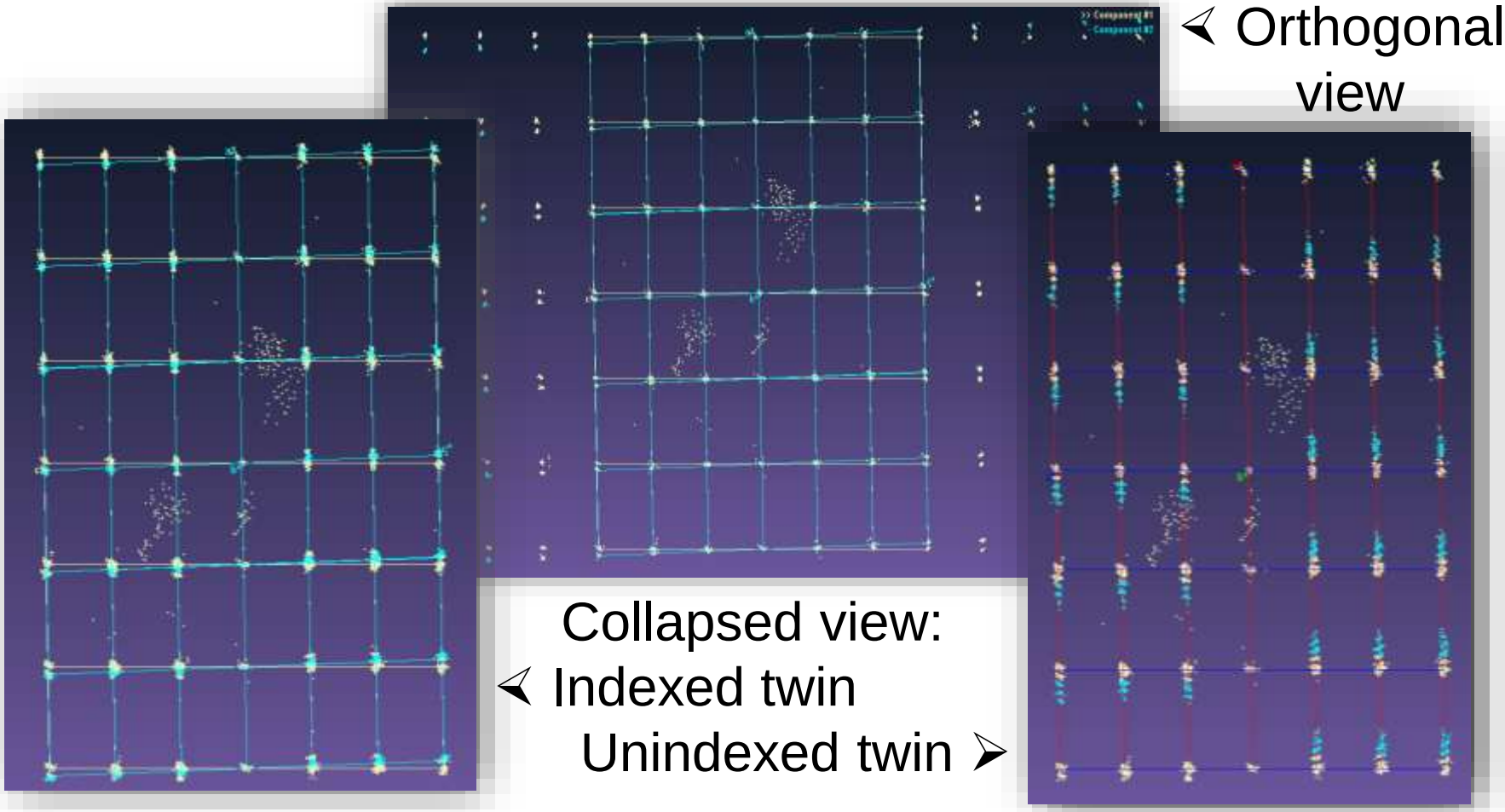
Ewald^{Pro} Collapse view

Collapse peak view – twin example



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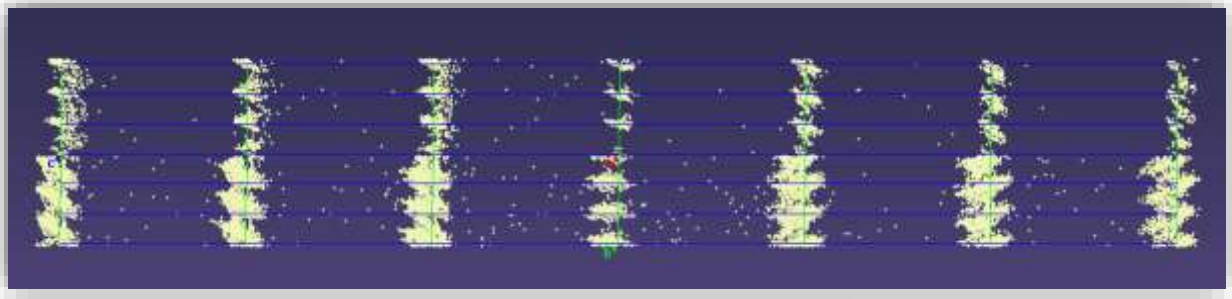
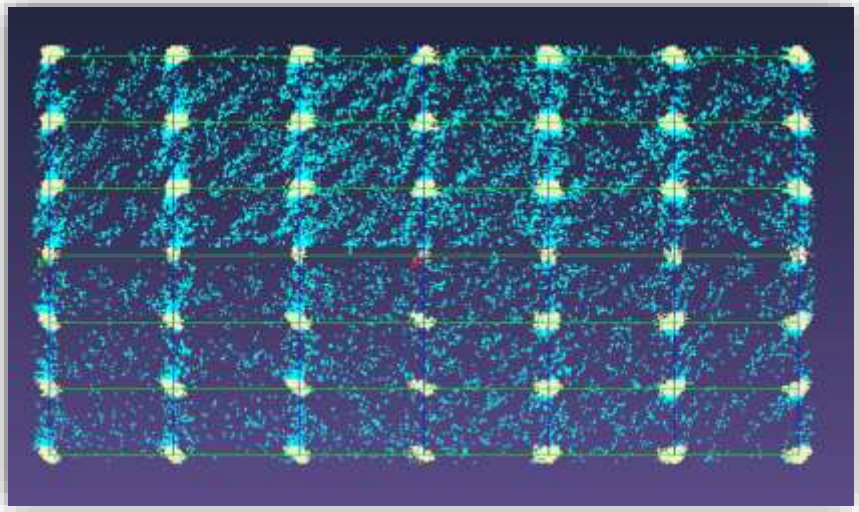
Ewald^{Pro} Collapse view

Collapse peak view – other examples





moving crystal

multicrystal

incommensurate

Rigaku
oxford diffraction

Data reduction

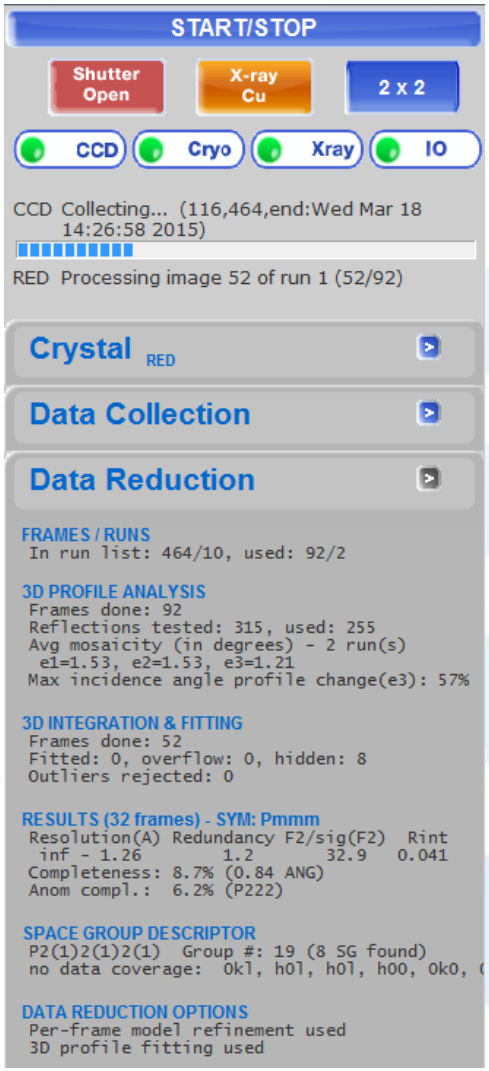
During experiment - concurrent data processing

- In most cases provides good, close to optimal results

- Features improving data quality:

  - Robust prediction model refinement

  - Selection of background evaluation mode



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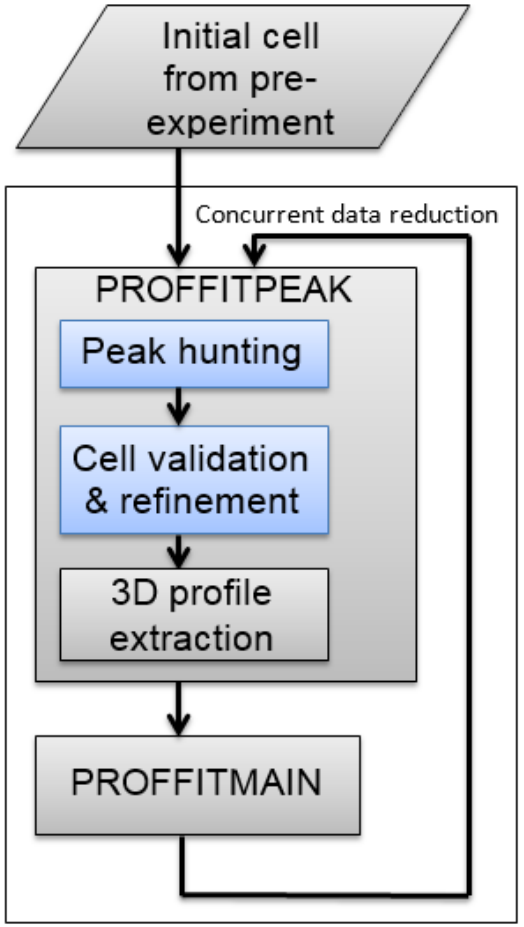
Data reduction

Concurrent data processing - Robust cell / model refinement

- The key problem:
  - Inaccurate initial cell from pre-exp
  - Cell/Model can't predict well low/high theta
  - Misaligned/jumping sample
- Solution:

PROFFITPEAK module does standard peak-hunting and cell/orientation refinement before profile learning / analysis phase



Rigaku oxford diffraction

Data reduction

Concurrent processing - Automatic selection of background

Average background level > threshold

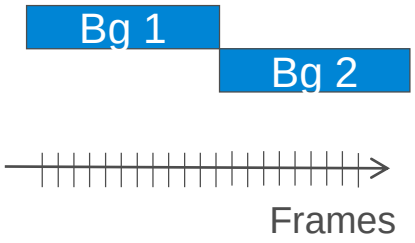
No

Yes

- Average background (Re>10 frames)

- Background image estimated once per specified frame range

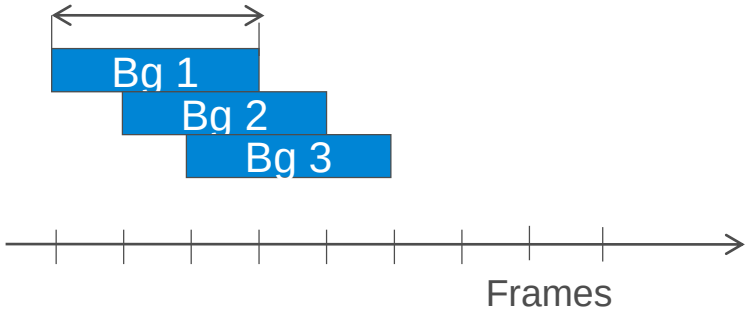
Re = Fr (default, >10 frames)



- Smart background

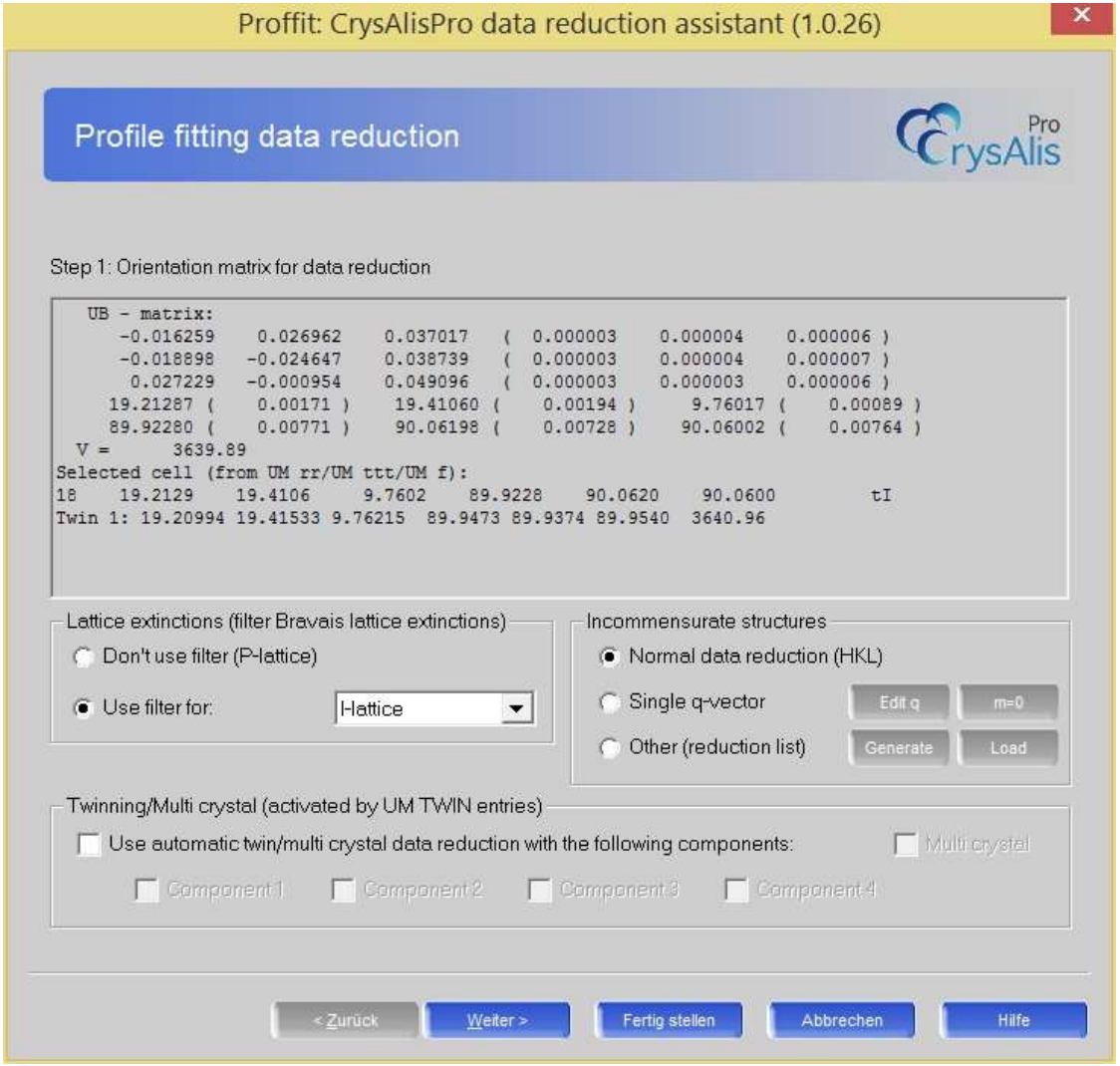
- Local background recomputed on every frame and fitted individually for every spot

Frame range: 1 (default), 3 or more available through the wizard



Rigaku oxford diffraction

Data reduction
Use of lattice filters



Rigaku oxford diffraction

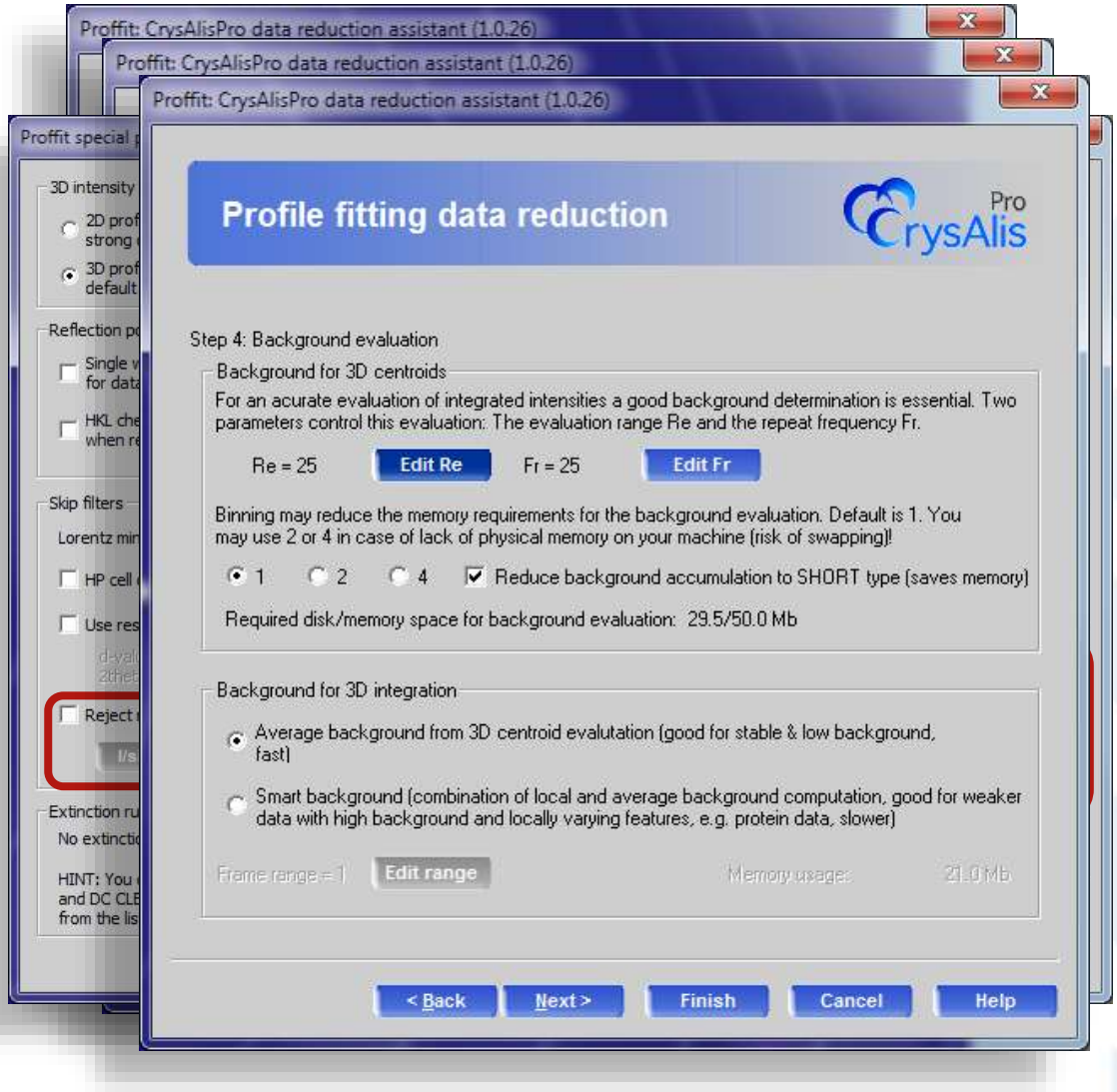
Data reduction
Data reduction wizard

Settings worth attention:

- Model refinement options

- Special parameters:
  - Integration mask size
  - Bad profile filter

- Background options



Rigaku
oxford diffraction

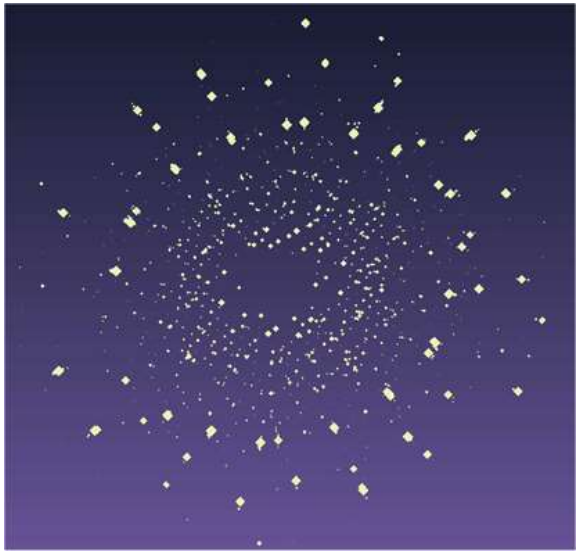
Data reduction
3D profile fitting

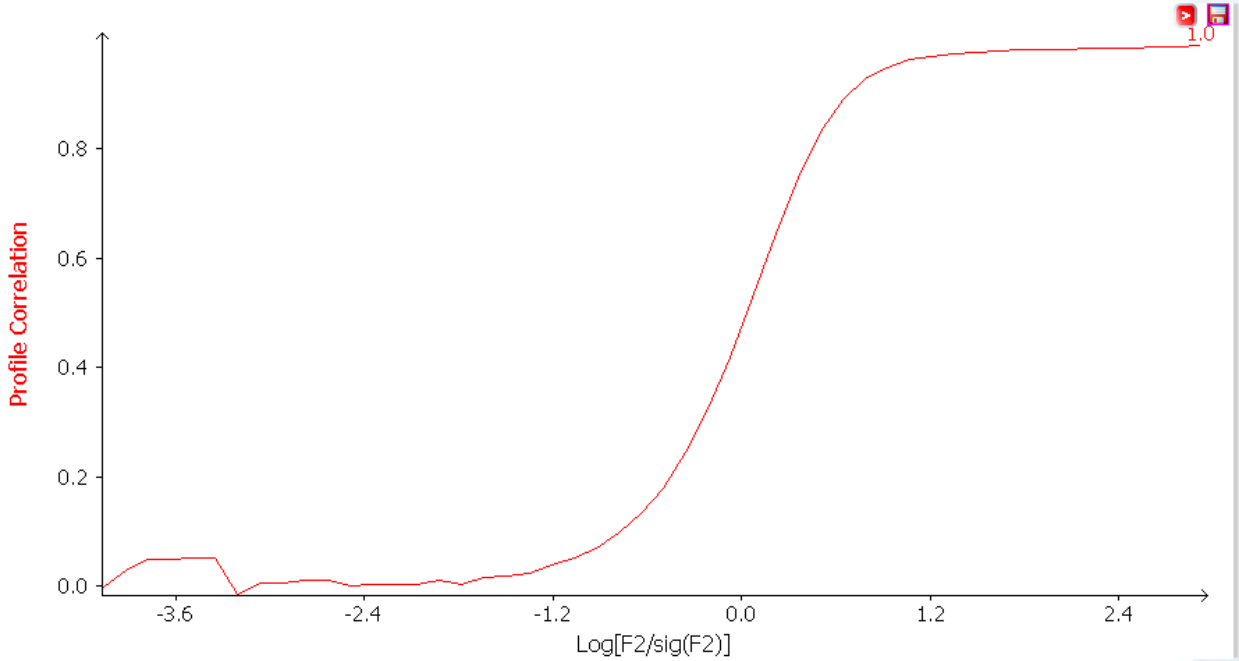
- Distorted rotation method data is mapped to ‘Kabsch-space’. Similar like XDS, but more complex
- Strong reflection data serve as reference profile. No shape assumption is made!
- All data is profile fitted to the ‘nearby’ reference profile. For strong data this means summation, for weak filtering
- You may choose to take less/more than 4sig of reference profile

Data reduction

Special pars- outliers

- Filter intruders by correlation coefficient.
- All strong reflections are self similar.

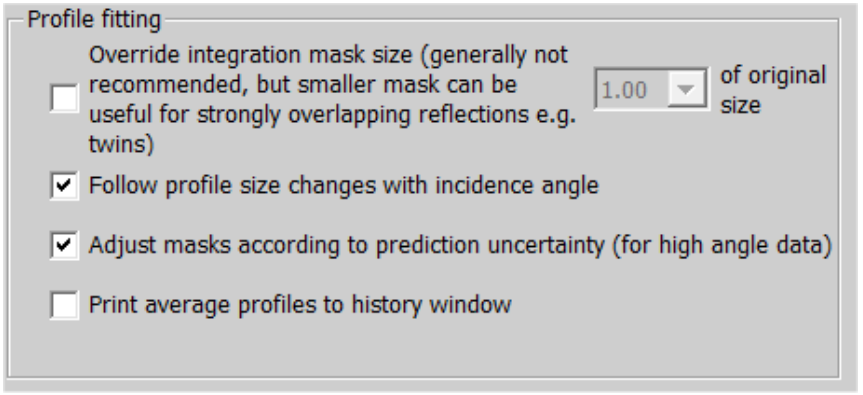




Rigaku
oxford diffraction

Data reduction

Special pars - incidence



Profile size analysis (per incidence angle)

Incidence angle (deg)	# of peaks	Average profile size - assuming Gaussian shape (in degrees) sig_e1 (stddev)	sig_e2 (stddev)	sig_e3 (stddev)
0-12.6	769	1.639 (0.304)	1.430 (0.233)	1.757 (0.880)
12.7-18.1	769	1.624 (0.354)	1.430 (0.242)	1.649 (0.875)
18.1-22.5	769	1.624 (0.357)	1.431 (0.258)	1.572 (0.828)
22.5-26.2	769	1.594 (0.369)	1.414 (0.258)	1.542 (0.839)
26.2-29.9	769	1.627 (0.372)	1.410 (0.282)	1.440 (0.736)
29.9-32.8	769	1.630 (0.364)	1.382 (0.255)	1.391 (0.719)
32.8-35.8	769	1.594 (0.341)	1.341 (0.267)	1.392 (0.708)
35.8-38.9	769	1.632 (0.349)	1.337 (0.266)	1.315 (0.594)
38.9-41.9	769	1.638 (0.330)	1.294 (0.269)	1.303 (0.659)
41.9-51.6	769	1.618 (0.323)	1.221 (0.270)	1.188 (0.610)
0-51.6	7690	1.622 (0.347)	1.369 (0.269)	1.455 (0.769)

Fitted profile normalization line parameters

e1 dimension: a=0.0022 b=0.99

e2 dimension: a=-0.0019 b=1.08

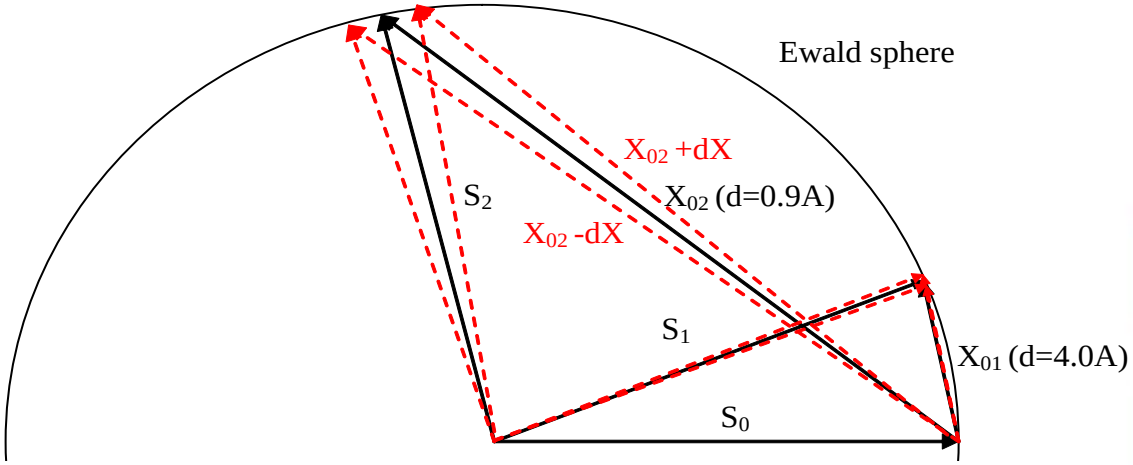
e3 dimension: a=-0.0136 b=1.46

Rigaku oxford diffraction

Data reduction

Prediction uncertainty – problem

- Problem lies in spot prediction uncertainty
- Higher inaccuracy at high theta



For profile size of 0.8 deg integration mask size is 8 pixels at incidence angle 0 deg (Atlas detector, 2x2 binning, at 55 mm)

Detector theta (deg)	Std dev of misprediction (deg)	Std dev of misprediction (pix)	Max misprediction (pix)
11	0.014	0.13	0.78
24	0.02	0.2	1.2
40	0.025	0.25	1.5
111	0.04 – 0.08	0.4 – 0.8	2.4 – 4.8

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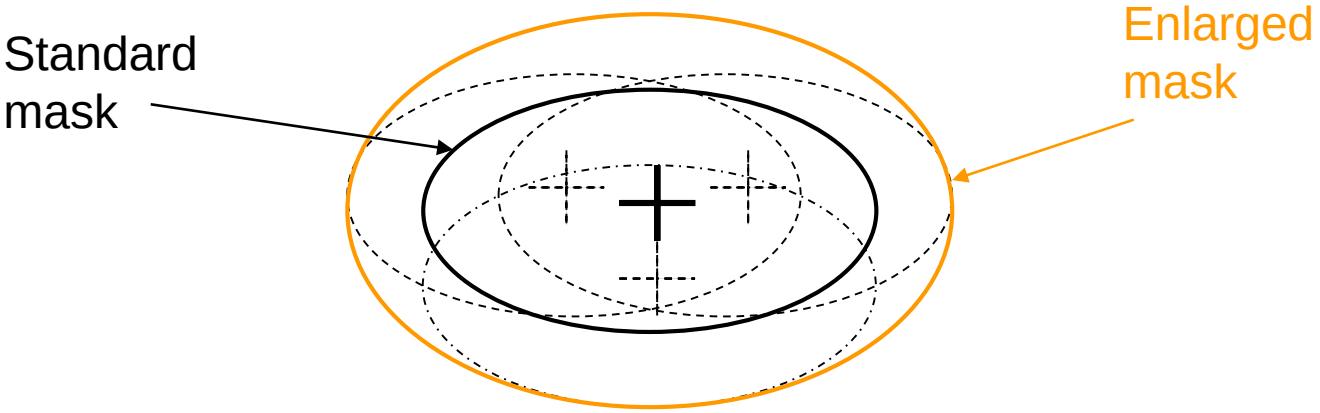
Data reduction
Prediction uncertainty – solution

- Estimate prediction uncertainty at given theta

Prediction accuracy statistics (in degrees)

		Average prediction error (in degrees)		
Resolution	# of peaks	delta_e1 (stddev)	delta_e2 (stddev)	delta_e3 (stddev)
1.35-1.22	82	0.002 (0.020)	0.001 (0.013)	0.003 (0.170)
1.22-1.14	82	-0.002 (0.025)	0.009 (0.016)	0.020 (0.165)
1.14-1.08	82	0.003 (0.024)	0.004 (0.020)	0.020 (0.175)
1.08-1.04	82	-0.012 (0.034)	-0.002 (0.021)	-0.026 (0.153)
1.04-0.99	82	0.001 (0.026)	-0.003 (0.021)	-0.018 (0.153)
0.99-0.95	82	-0.007 (0.033)	-0.005 (0.030)	-0.004 (0.147)
0.95-0.91	82	-0.005 (0.038)	-0.009 (0.029)	-0.001 (0.132)
0.91-0.87	82	-0.008 (0.038)	-0.015 (0.041)	-0.002 (0.127)
0.87-0.84	82	0.006 (0.038)	-0.012 (0.041)	-0.016 (0.106)
0.84-0.80	73	0.005 (0.051)	0.017 (0.087)	0.002 (0.103)
1.35-0.80	811	-0.002 (0.034)	-0.002 (0.038)	-0.002 (0.146)

- Enlarge integration mask according to prediction uncertainty



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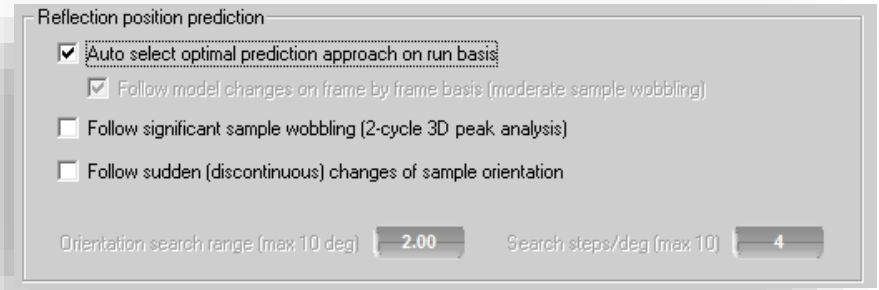
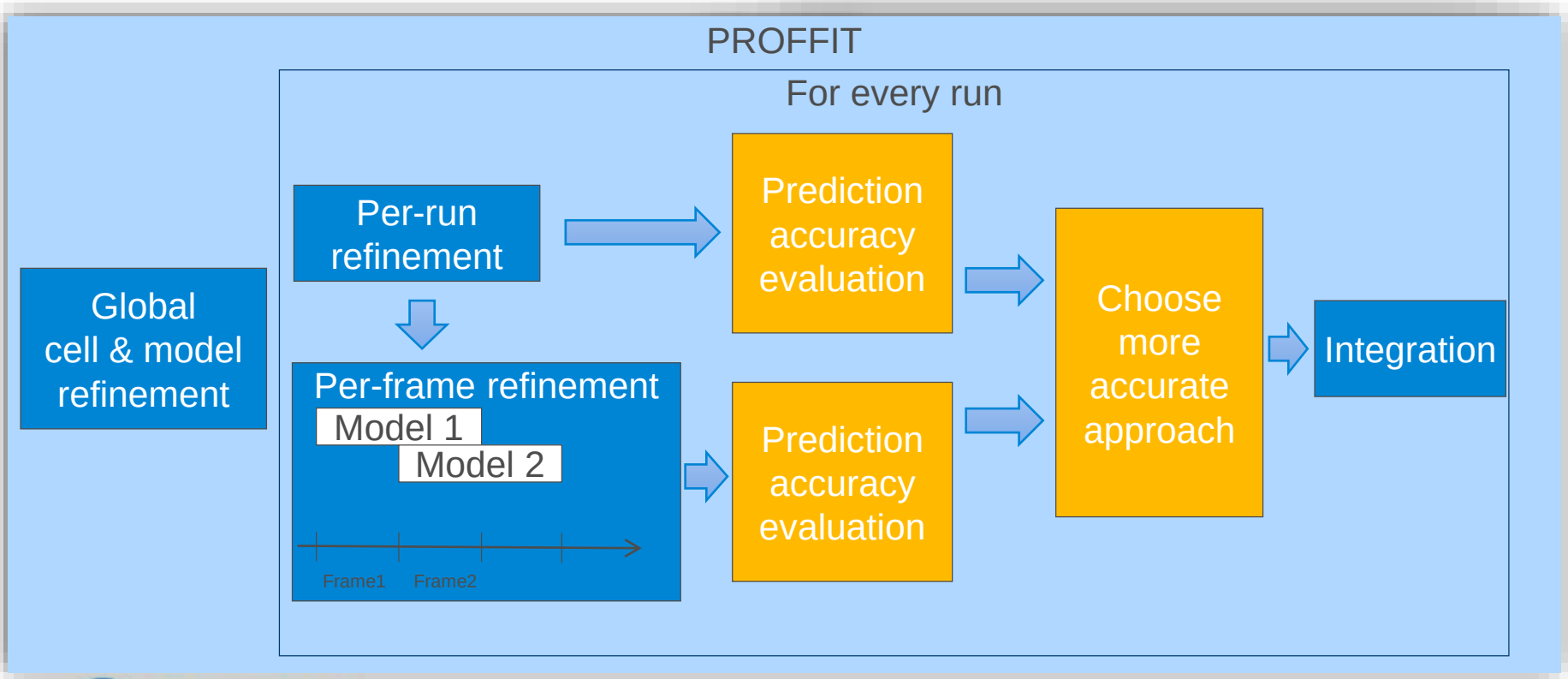
Data reduction
Model refinement options

No need to decide
– program does it for you!





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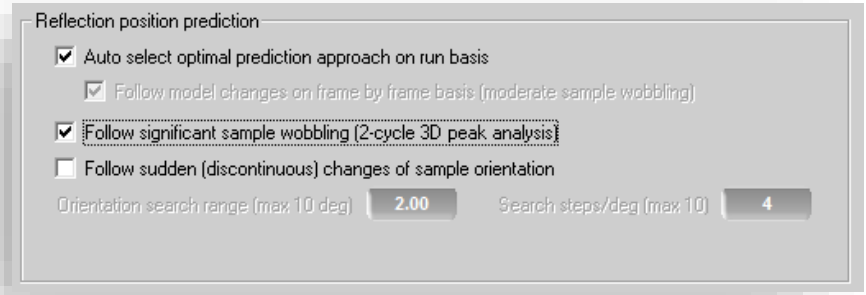
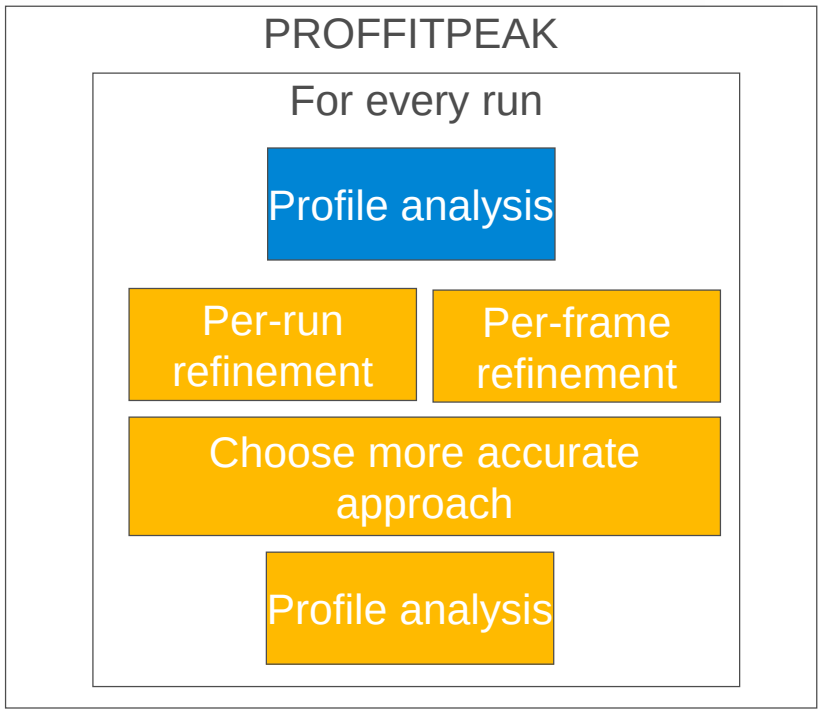
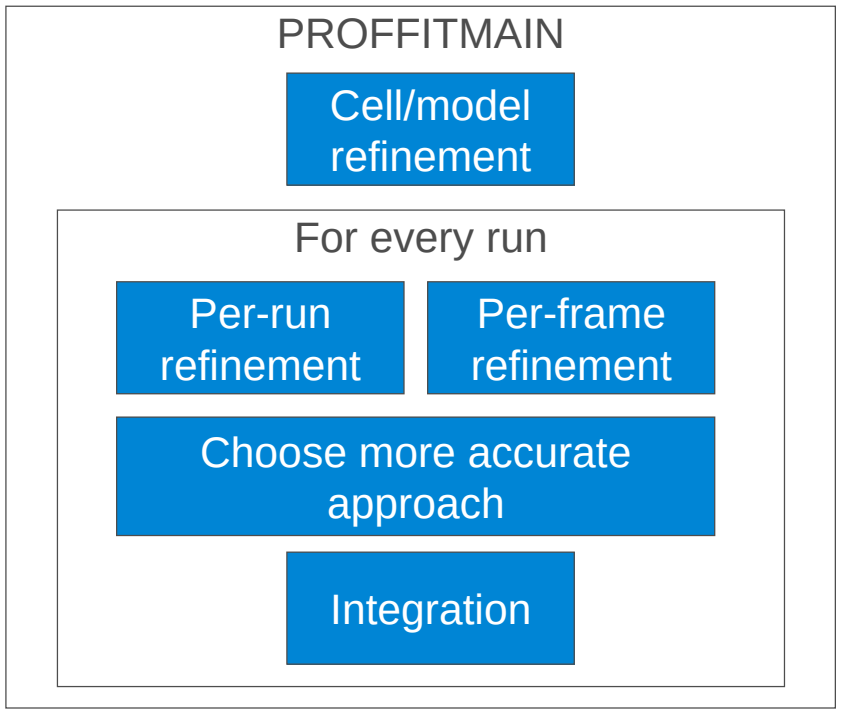
Data reduction

Model refinement options



- 2-cycle PROFFITPEAK
- Covers more difficult “wobbling” cases





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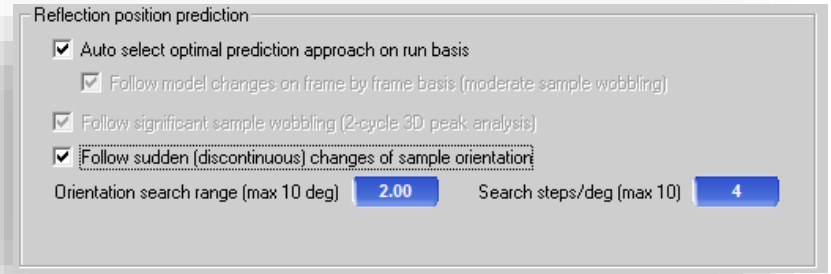
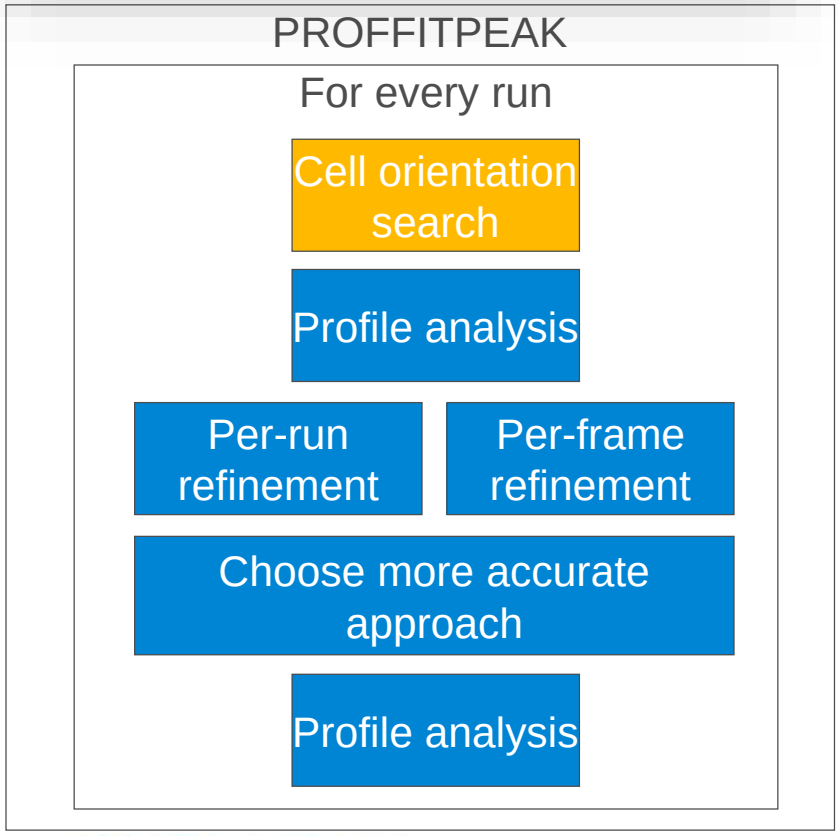
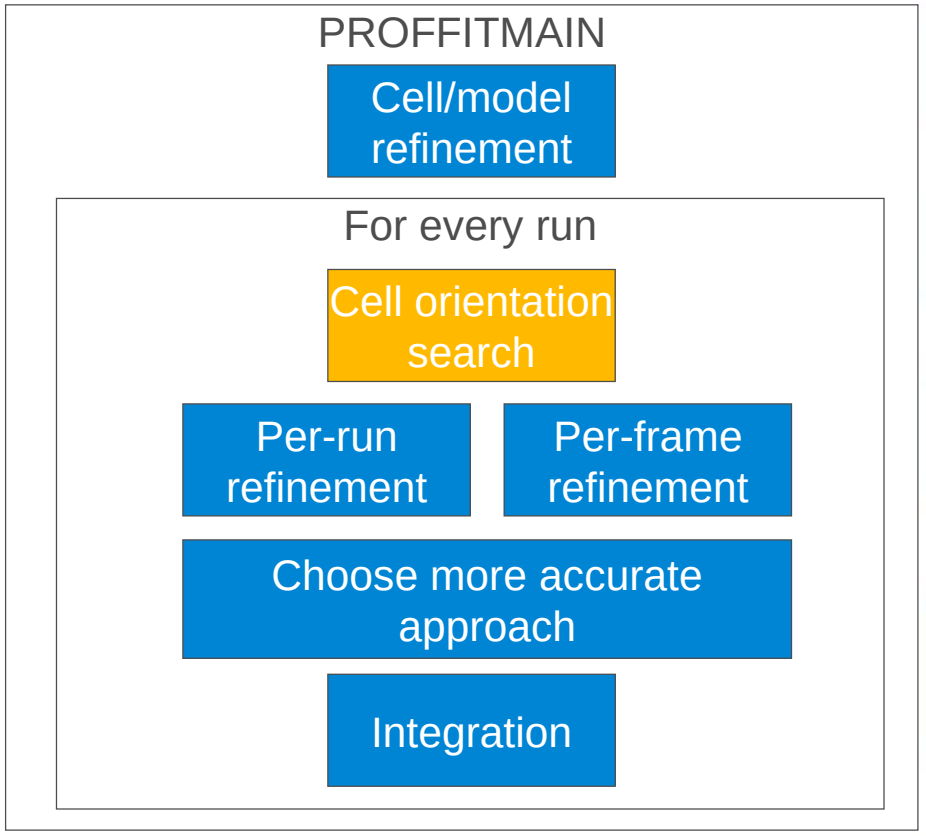
Data reduction

Model refinement options



- Model refinement with matrix orientation search
- For discontinous sample jumps (LT, flexible holder, not fixed properly, etc.)





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Manual Data Reduction

Sample slippage example

- Superficially gives impression of twin
  - Twin indexing matches 96.8% of reflections

TWIN ANALYSIS

Component	Ratio	Isolated	Overlapped
1	0.37	1676	24
2	0.63	1690	24

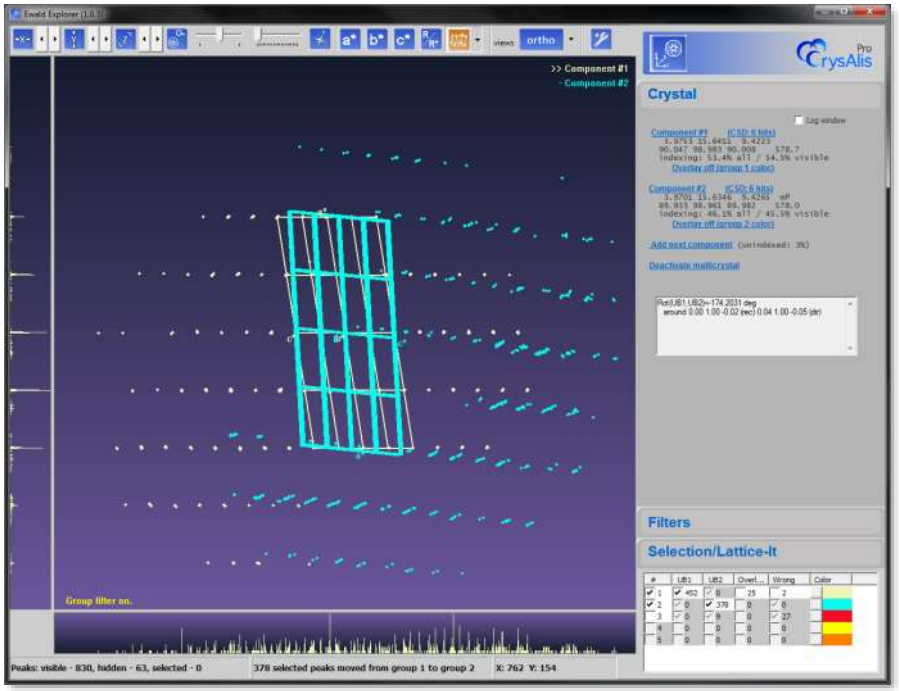
DECOMPOSED TWIN DATA STATISTICS (<0.80 overlap)

Component	Redundancy	F2/sig(F2)	Rint
1	1.5	9.7	0.245
2	1.5	7.0	0.658

Overlap limit for HKLF4 export: 0.80

TWIN HKLF5 STATISTICS FOR OVERLAPPED OBS

Components	Redundancy	F2/sig(F2)	Rint
1,2	1.3	24.8	0.223



… but twin integration doesn't help

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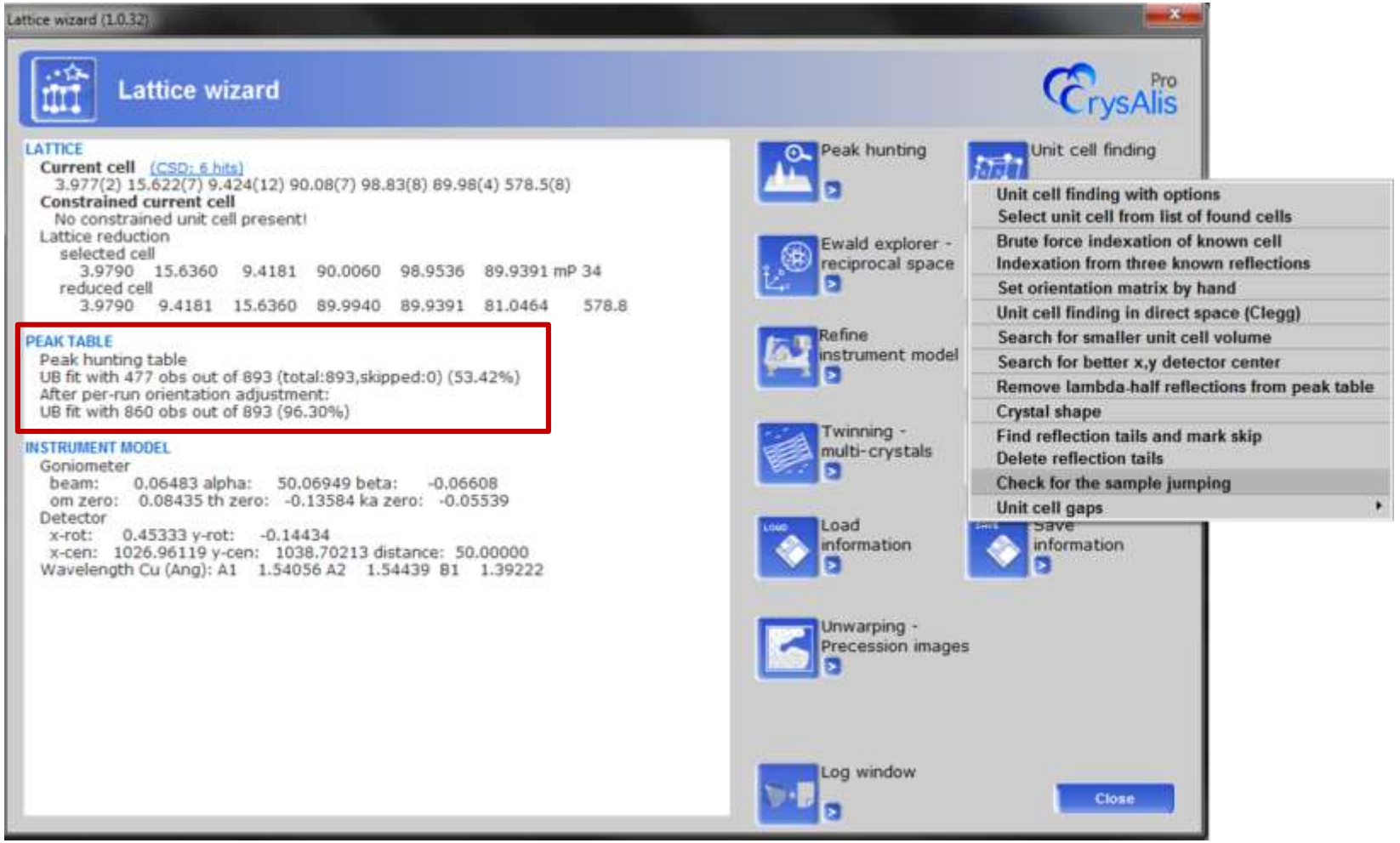
Manual Data Reduction

Sample slippage example



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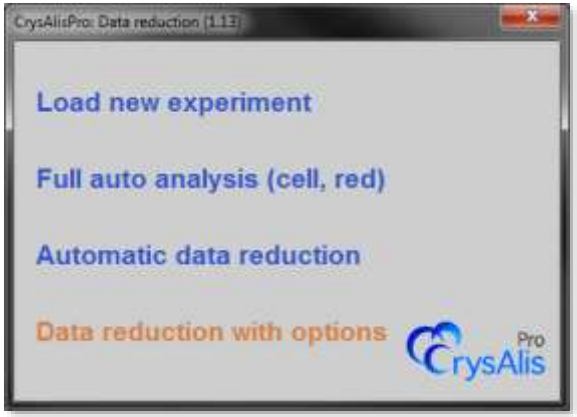
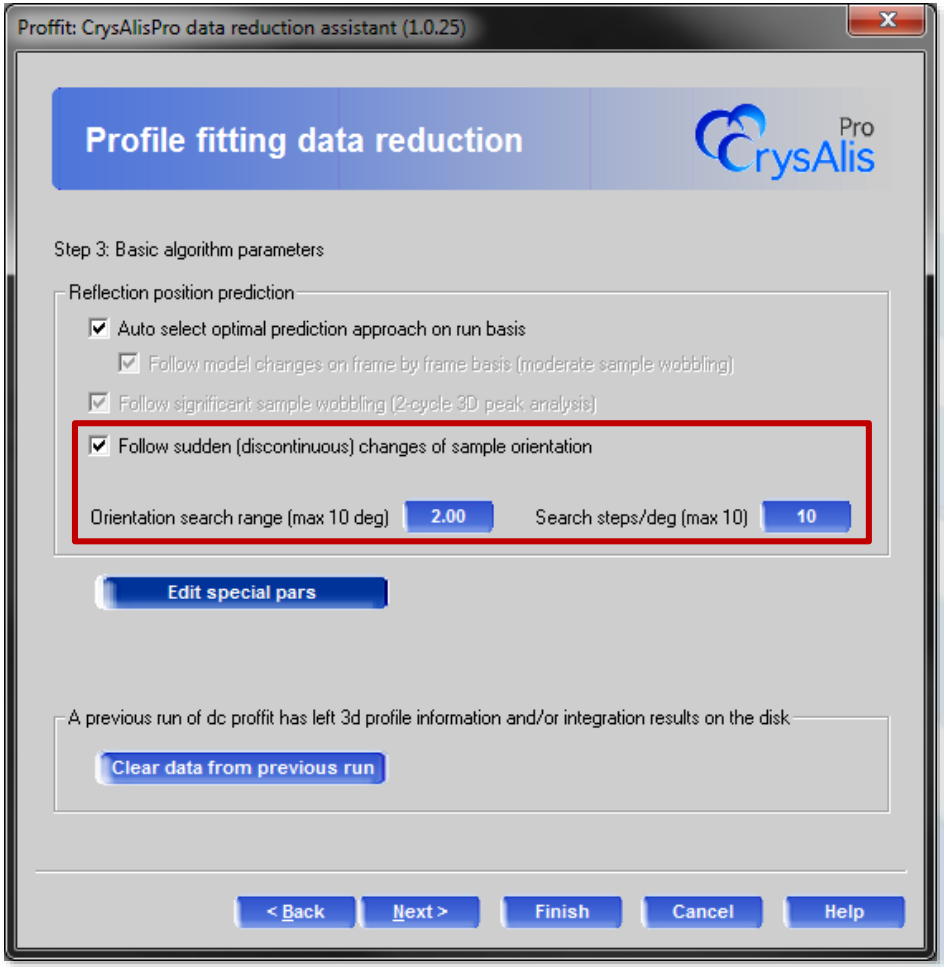
Manual Data Reduction

Sample slippage example






```
RESULTS (466 frames) - SYM: P2/m (b-unique)
 Resolution(A) Redundancy F2/sig(F2)  Rint
  inf - 0.80        1.5       22.4    0.016
  inf - 0.84        1.5       23.2    0.016
 Completeness: 98.4% (0.84 ANG)
```

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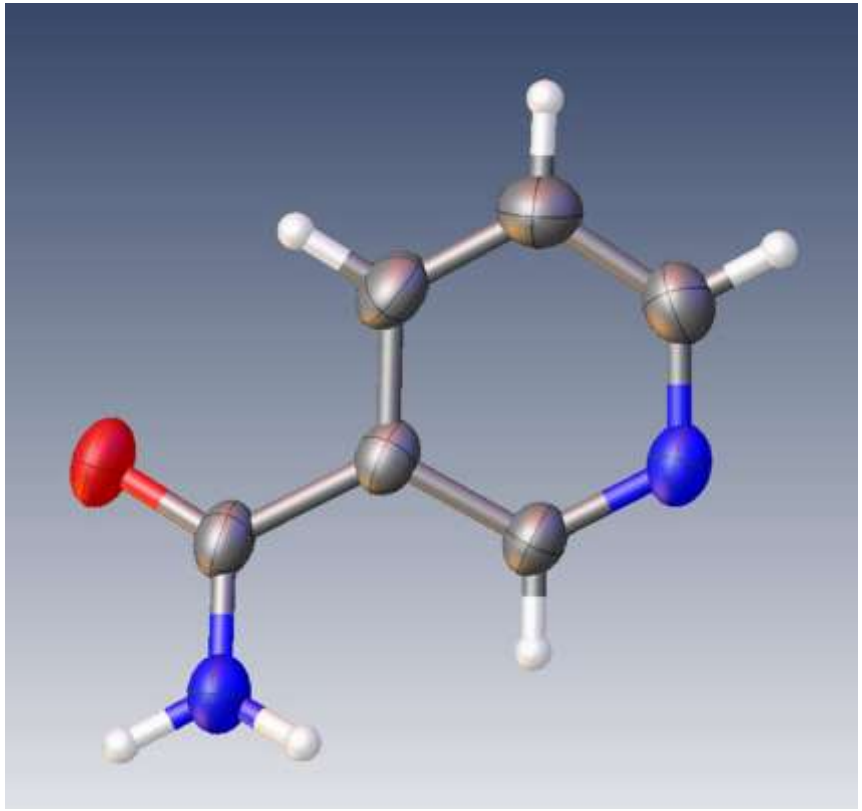
Manual Data Reduction

Sample slippage example



	No slip	Intentional sample slip	
	Reference data	Slip Data (Pre-Treatment)	Slip Data (Post-Treatment)
R_{int} (%)	1.6	14.7	1.6
I/σ	22.0	5.0	22.9
R_1 (%)	3.32	43.88	3.46
Comp (%)	98.5	95.2%	98.4%

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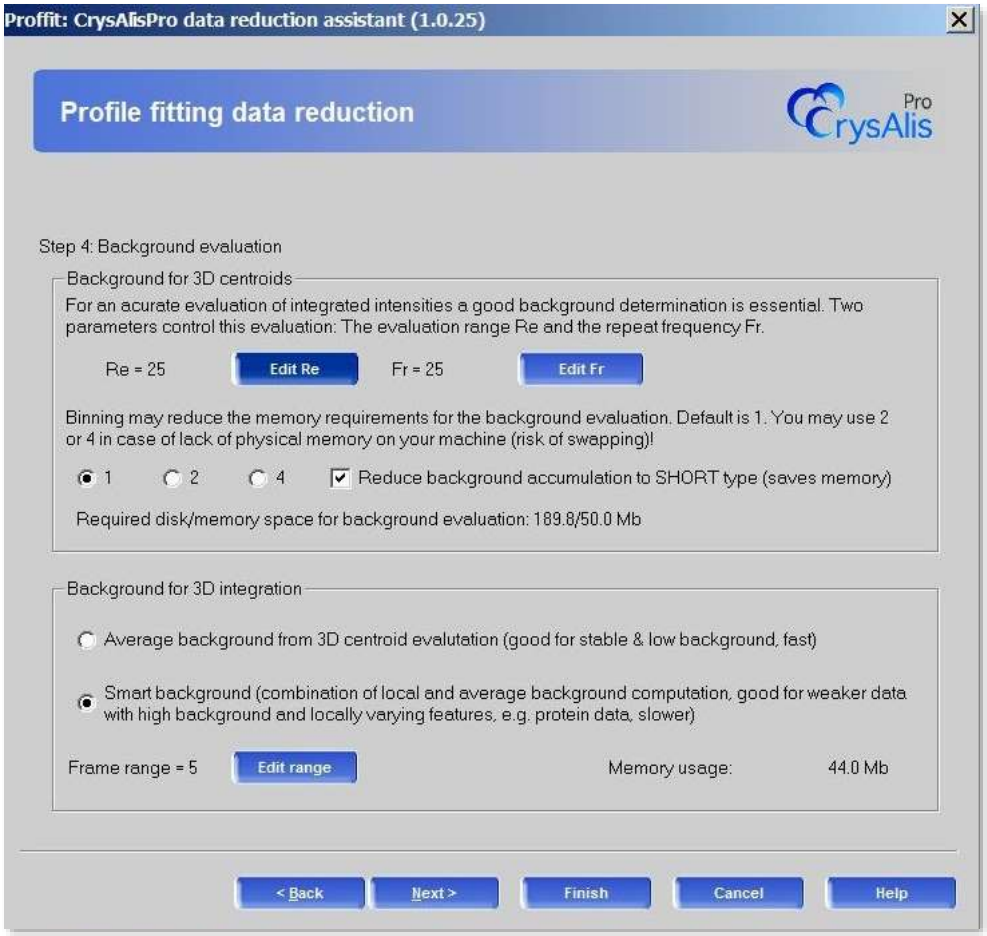
Manual Data Reduction

Background correction



Choice of background correction:

- Average background
  - Define range and frequency
- Smart background
  - Combination of local and average background
  - Improves statistics (I/σ) for samples with varying background features

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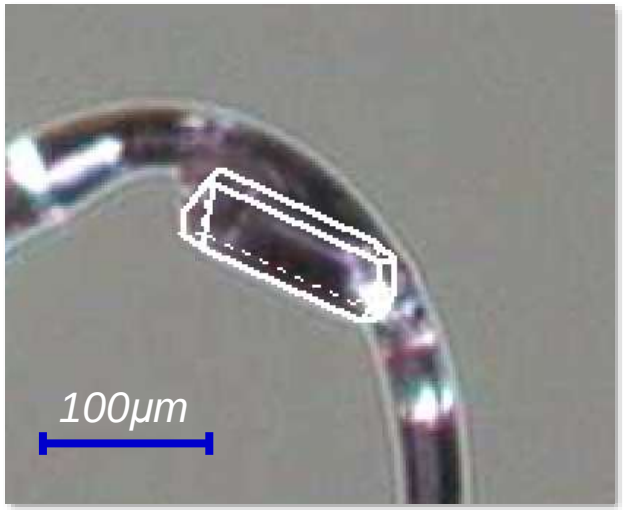
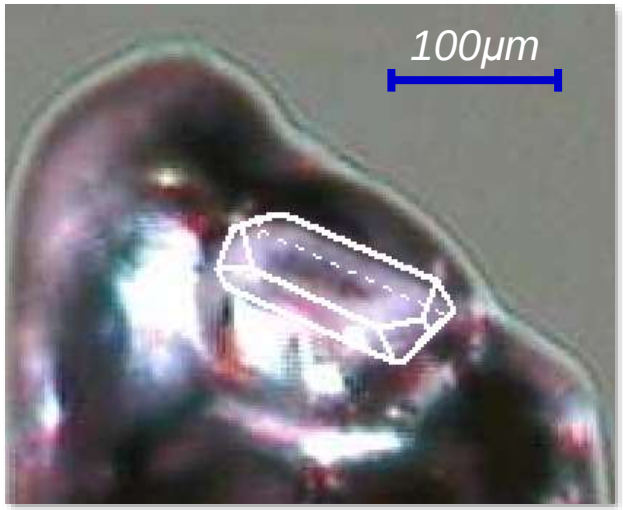
Manual Data Reduction

Background correction

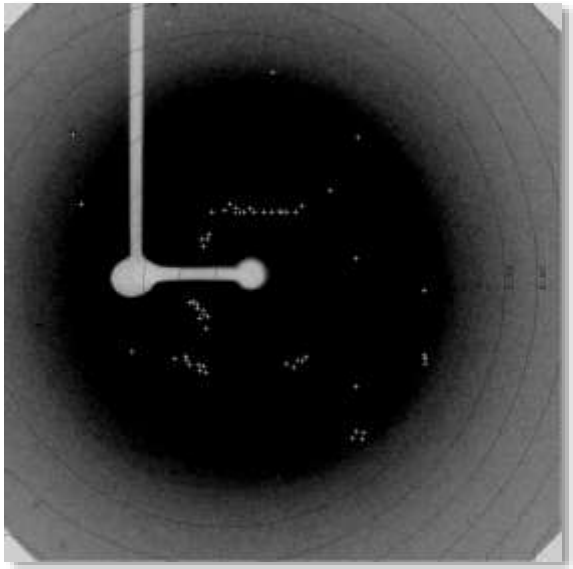


Well-mounted sample



Intentionally badly-mounted sample

Standard peak-hunting produces many non-lattice peaks.



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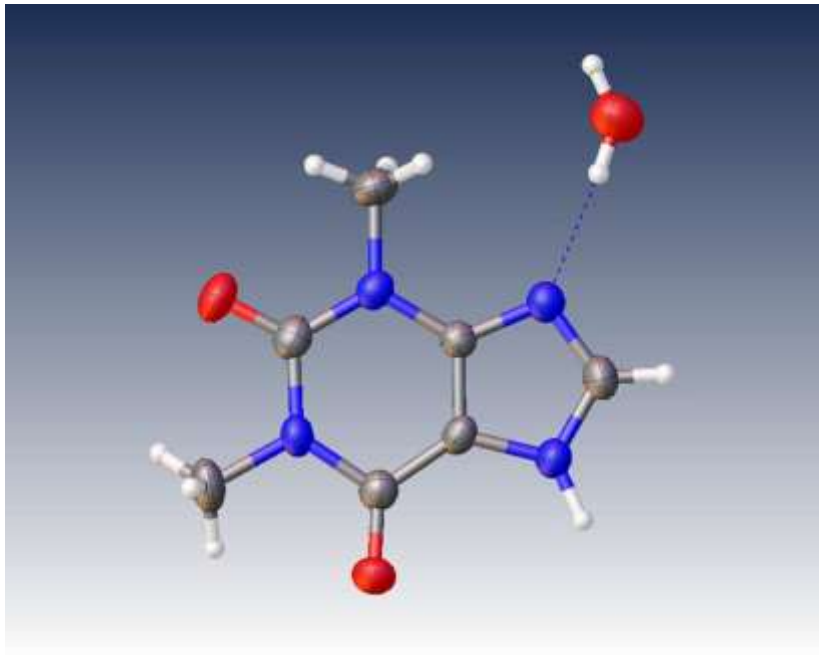
Manual Data Reduction

Background correction



	Well-mounted	Badly-mounted	
	Reference Data	Auto analysis	Smart Background
Time	3h 8m	16h 18m	16h 18m
Diff. Limit	0.92	1.41	0.97
R_{int} (%)	3.1	14.4	5.8
I/σ	13.5	3.0	7.8
R_1 (%)	5.28	-	6.22
Comp (%)	99.5	99.5	99.5

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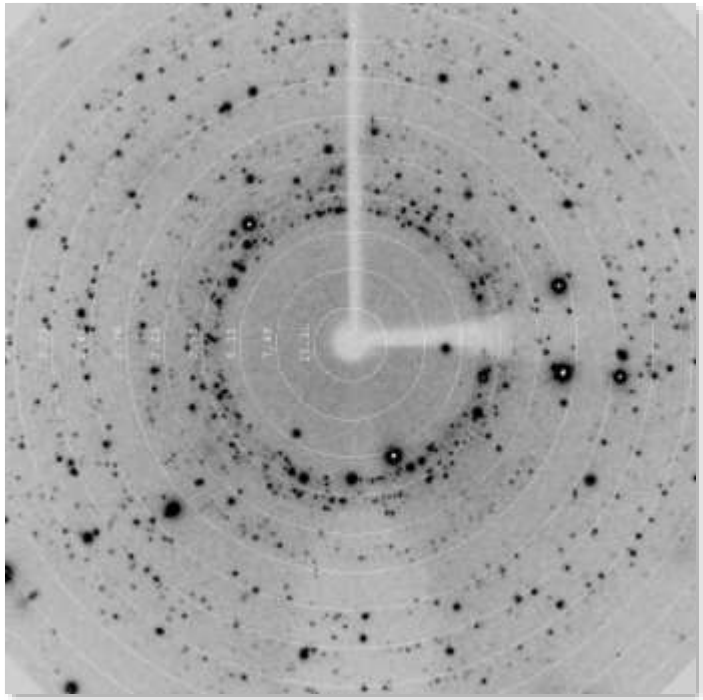
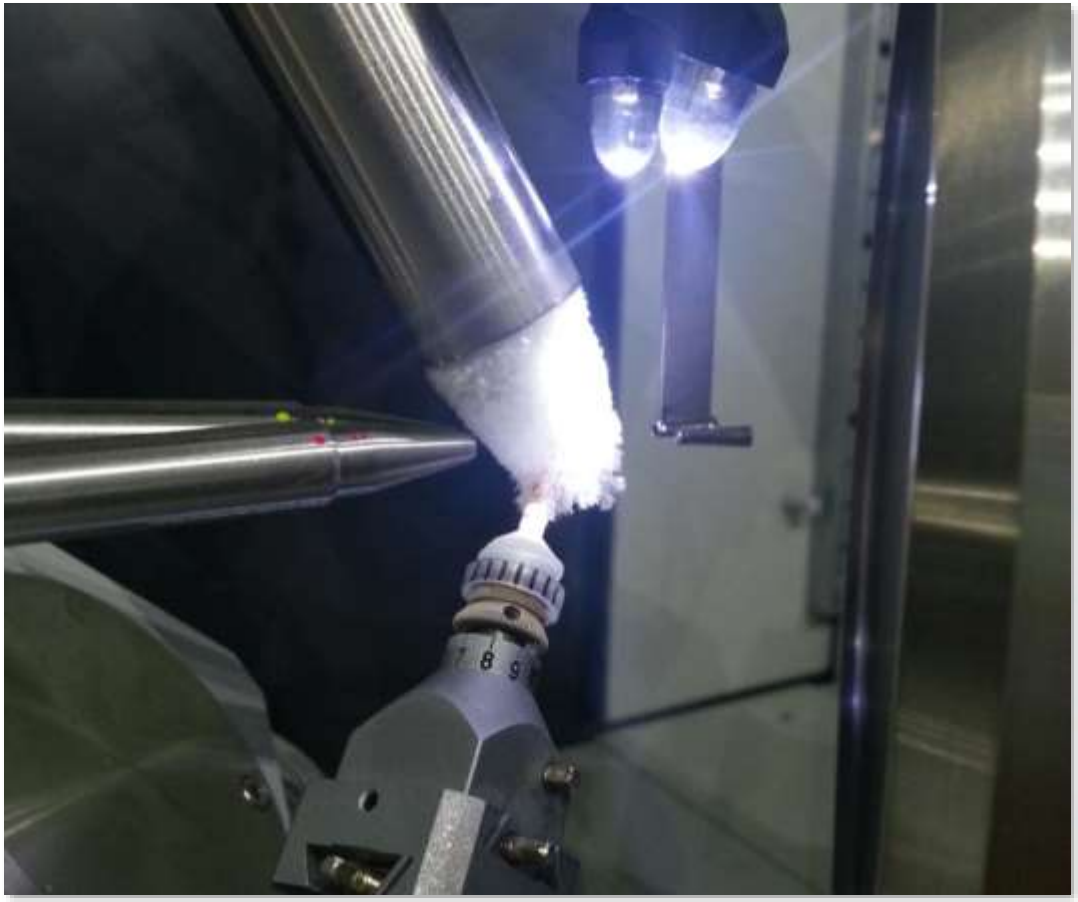
Manual Data Reduction

Bad profile rejection



Simulation of cryo-failure
(shield flow turned off)



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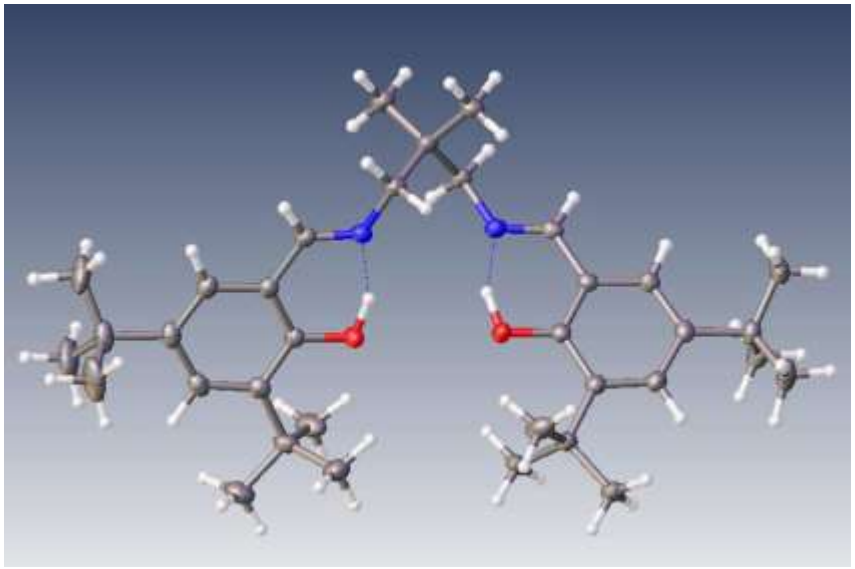
Manual Data Reduction

Bad profile rejection



	No ice	Large ice build-up		
	Reference Data	Auto analysis	d range and run Filtering	**Bad profile filtering**
R_{int} (%)	2.6	10.5	3.2	4.0
I/σ	17.7	8.4	14.0	12.7
R_1 (%)	3.83	6.11	4.11	4.50
Comp (%)	99.9	99.9	92.6	98.6

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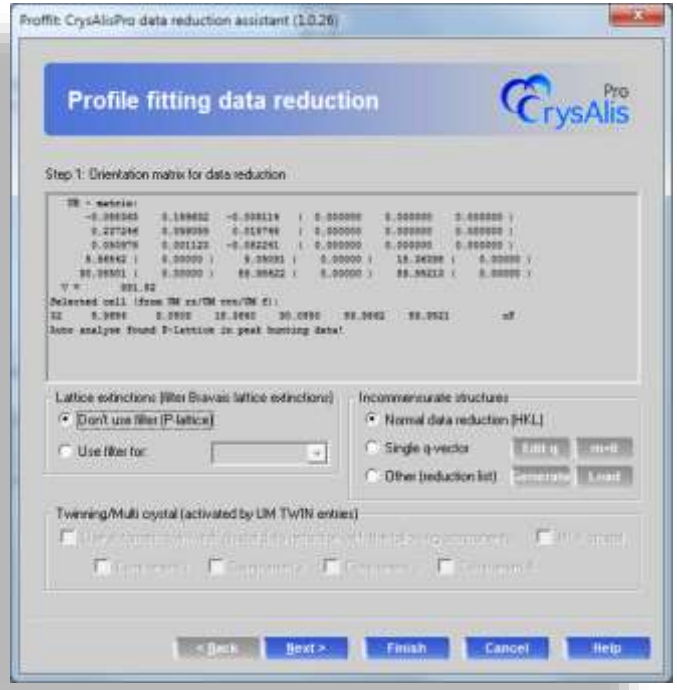
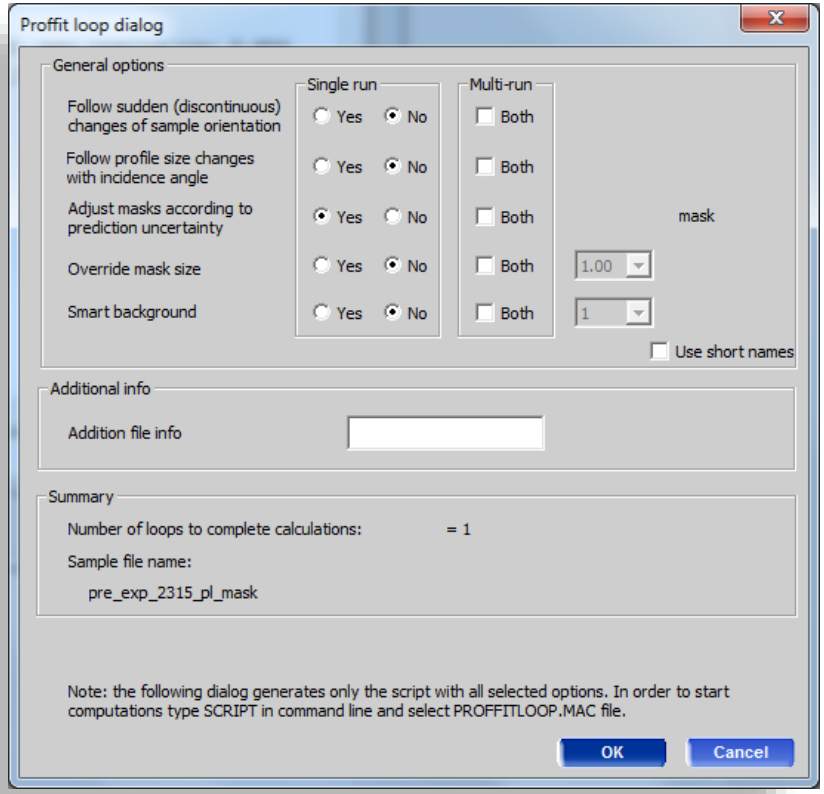
Manual Data Reduction

XX PROFFITLOOP - ultimate tool

- Not satisfied with the results, consider trying different option combinations using PROFFITLOOP tool





Caution! This tool may run for a long time and generate a lot of output files with gibberish names

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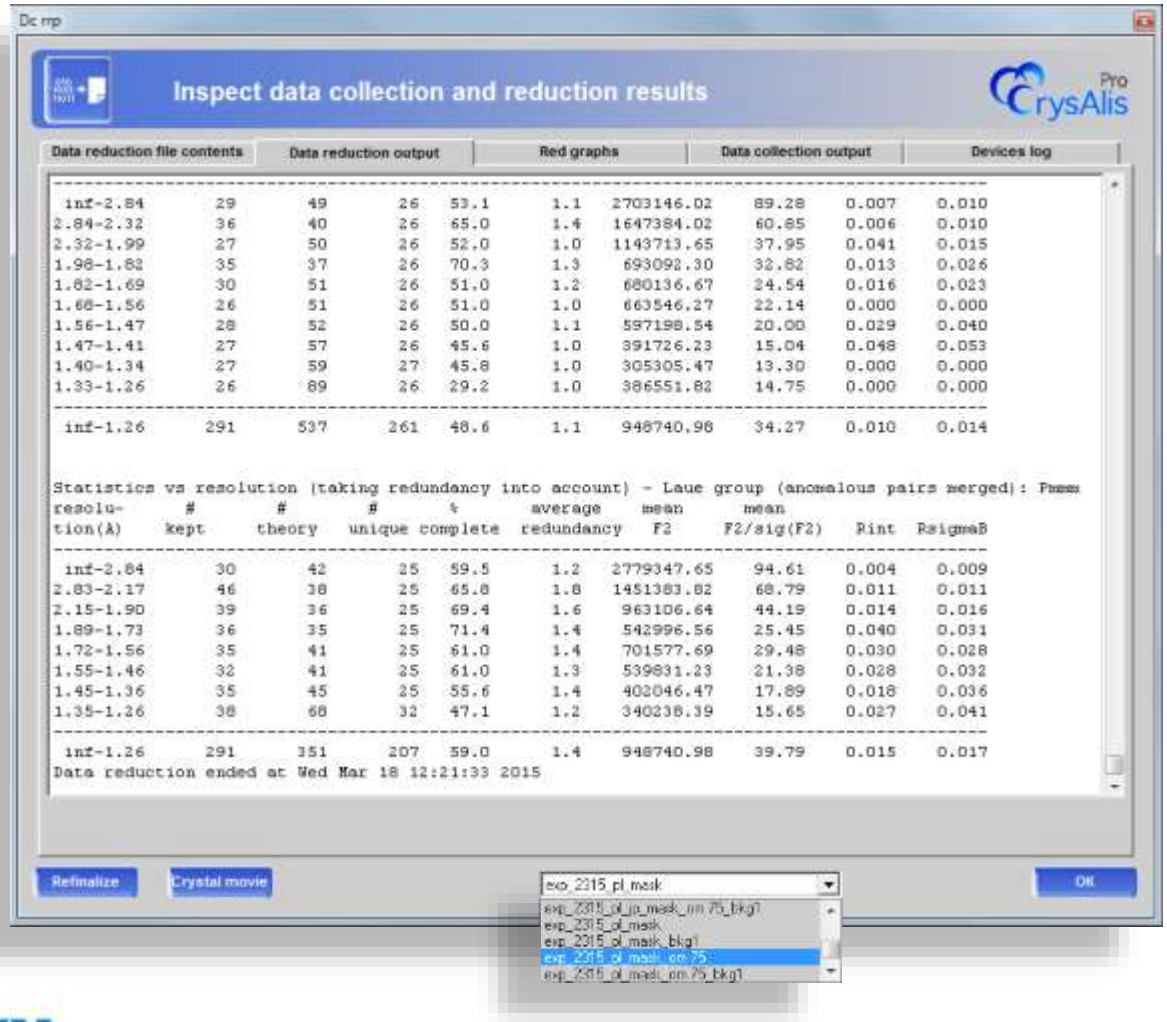
Manual Data Reduction

XX PROFFITLOOP - ultimate tool

- Afterwards browse the results in the finalizer window



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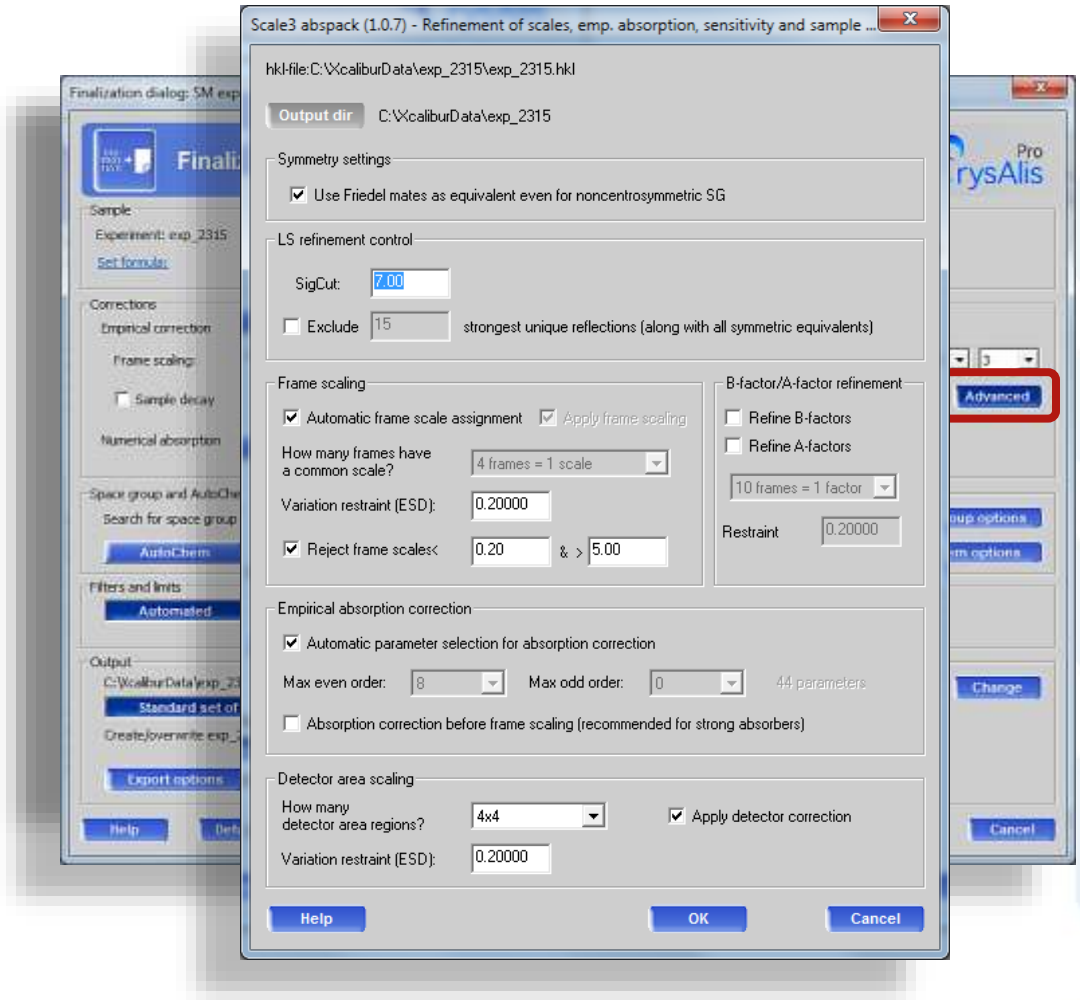
Post-integration empirical corrections

- Scaling
- Empirical absorption based on spherical harmonics
- Decay
- Detector sensitivity

Try manual settings!



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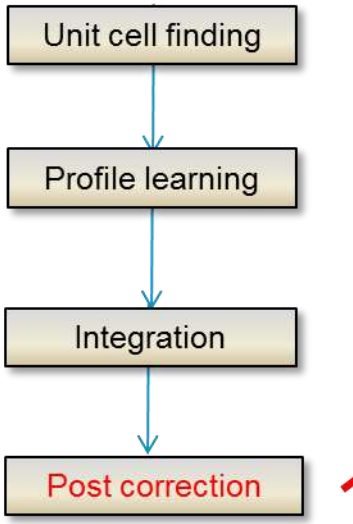
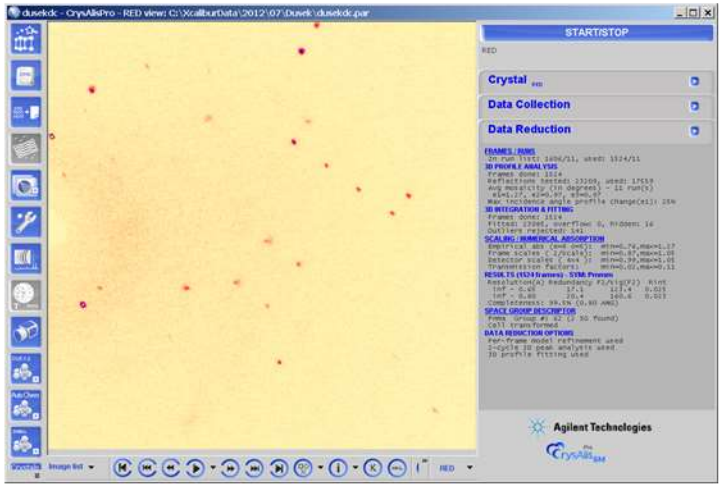
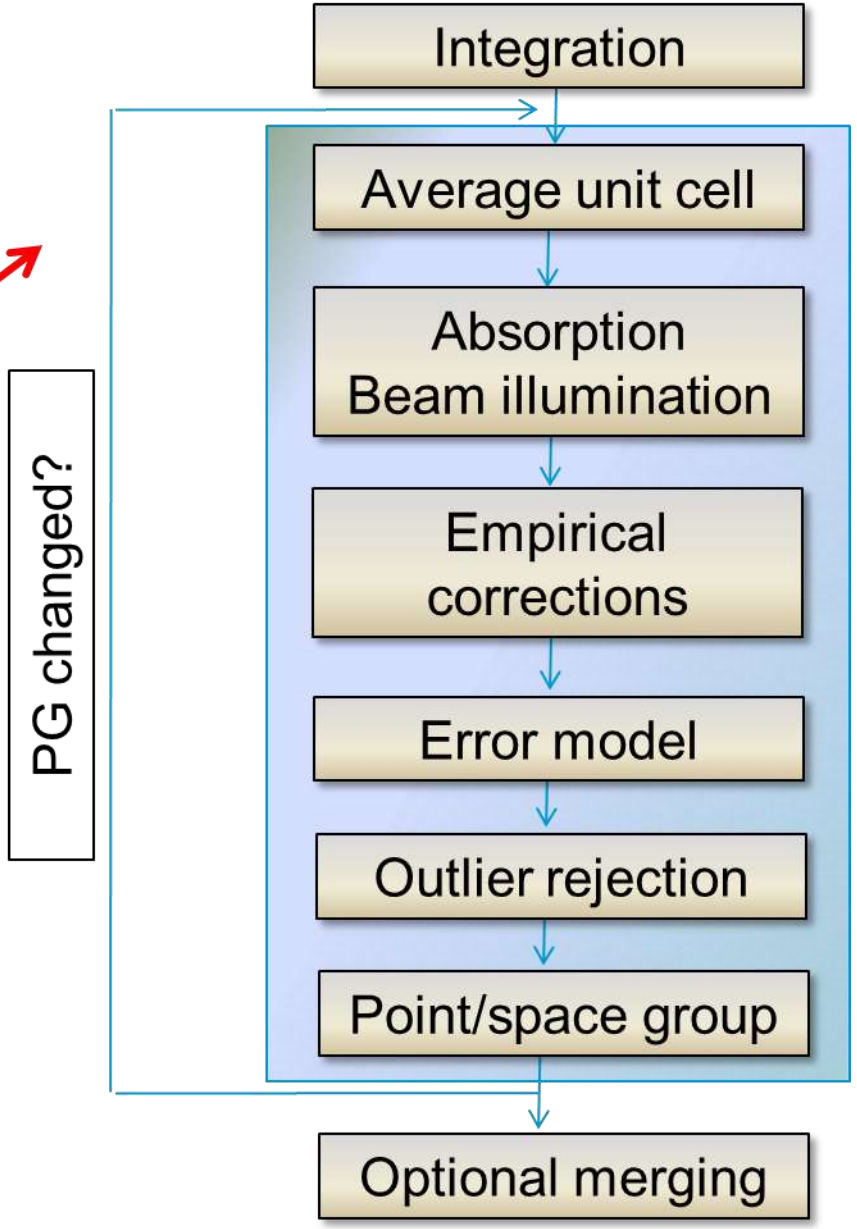
Remark on scaling of non-centro data







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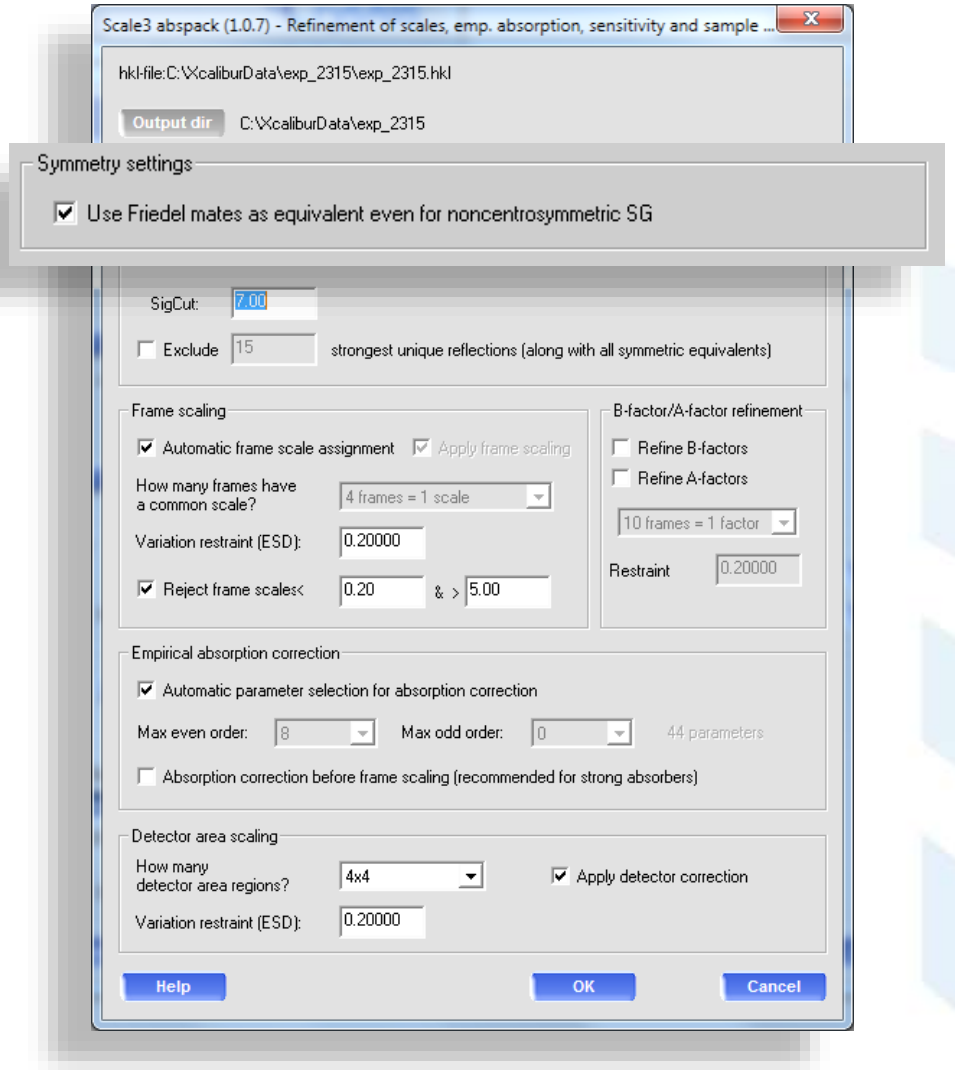
Remark on scaling of non-centro data

- Organic samples – Friedel pairs equivalent
- Samples with heavier atoms – scaling with Friedel pairs merged may destroy anomalous signal info
- Version 38 makes automatic decision based on provided formula (“heavy” means Si for Cu, Sc for Mo)



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Optimal data – hints at experiment time

- Centering/Sample choice/holder/amount of oil
- Low T: de-ice runs
- Absorption: make movie 1-6 deg
- Concurrent data red re-start
- Cu – Mo choice
- Collect redundant data
- Rather reduce scan width than increase dd
- Check your diffraction limit

Optimal data – hints at unit cell finding time

- Check for non-indexing reflections
  - Garbage (ice rings, powder), twin, sample jump
  - Re-run refine model
- Ewald
  - Use filters (intensity, lattice type) and groups
  - Use intensity view
- Check chemical formula unit cell consistency

Optimal data – hints at data reduction time

- Check for experiment artifacts (empty frames, trips)
- Apply Bravais lattice where obvious
- Special pars
  - Use bad reflection filter
  - Use reduced profile size if overlapping
  - Incidence correction, prediction accuracy
- Smart background on high background data
- xx proffitloop

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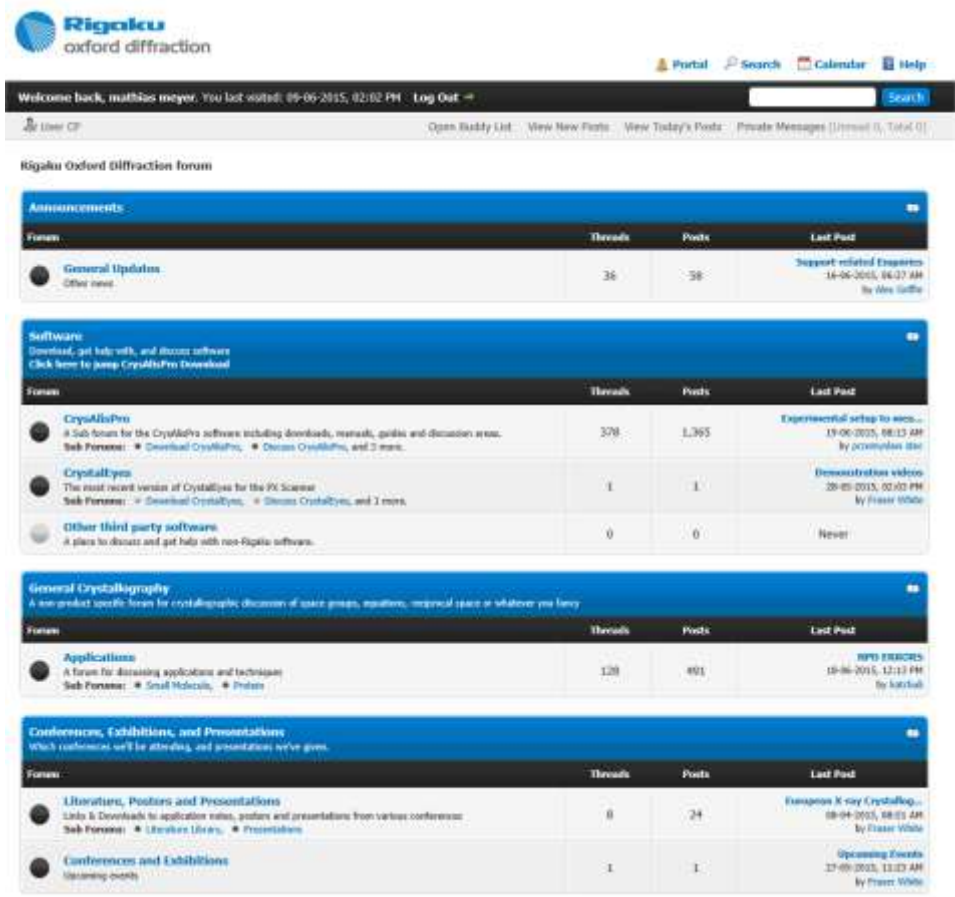
Optimal data – hints at data finalization time

- Hand set empirical parameters
- Use shape based absorption correction
- Apply filters carefully (e.g. Rint)
- Interactively decide space group
- Remove unnecessary data via d-value filter

Software Updates

- **CrysAlis^{Pro}** is frequently updated with fixes for known problems
- New features are introduced in annual major updates
- All updates are ***Free*** and available from our user forum, http://www.rigakuxrayforum.com
- ***Free*** multi-user, multi-site license



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Thank you for listening!

Find out more at

www.rigaku.com

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