RMS

Testing · Research · Consulting

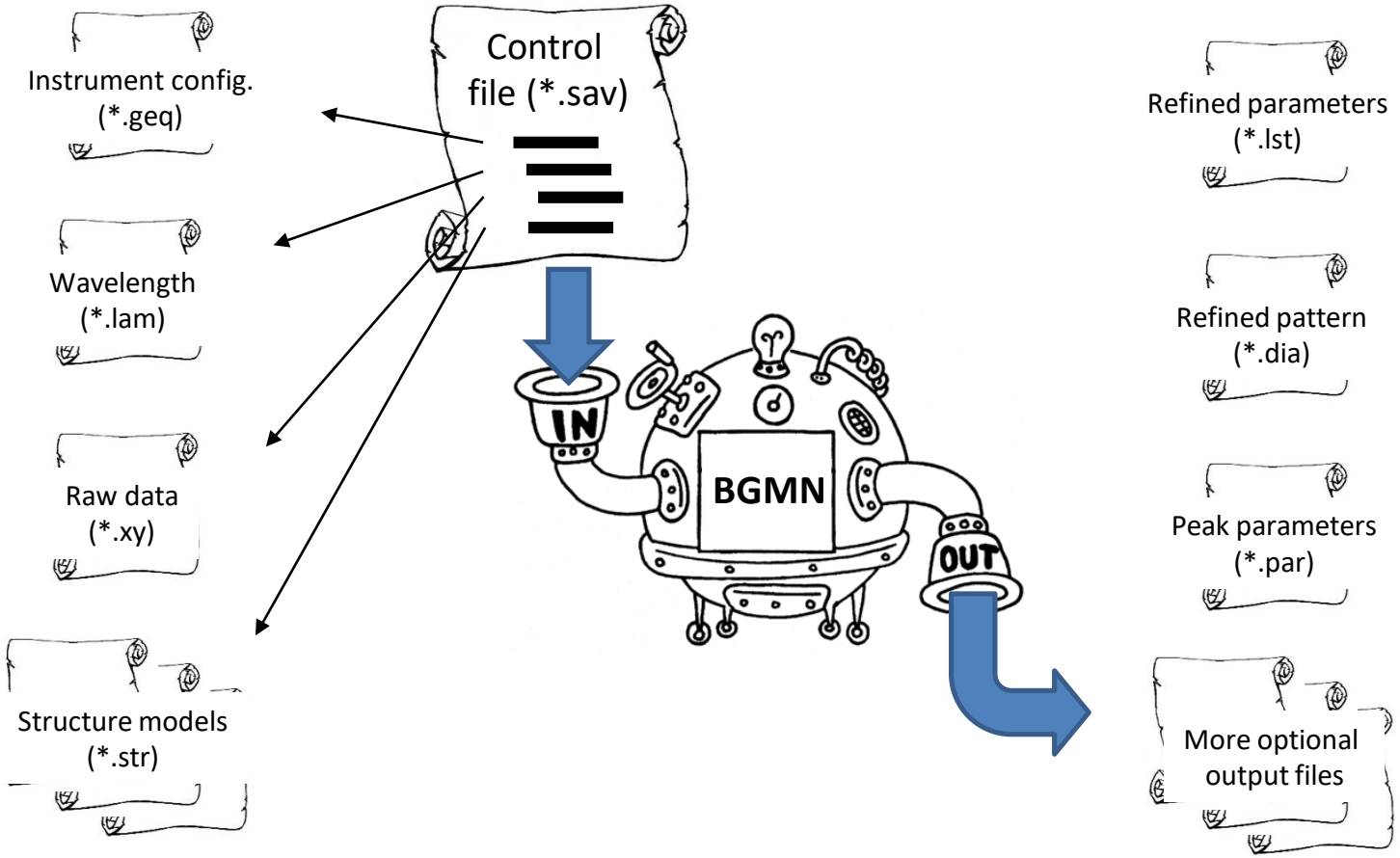
BGMN/Profex User Meeting 2019

Profex – A Graphical User Interface for BGMN

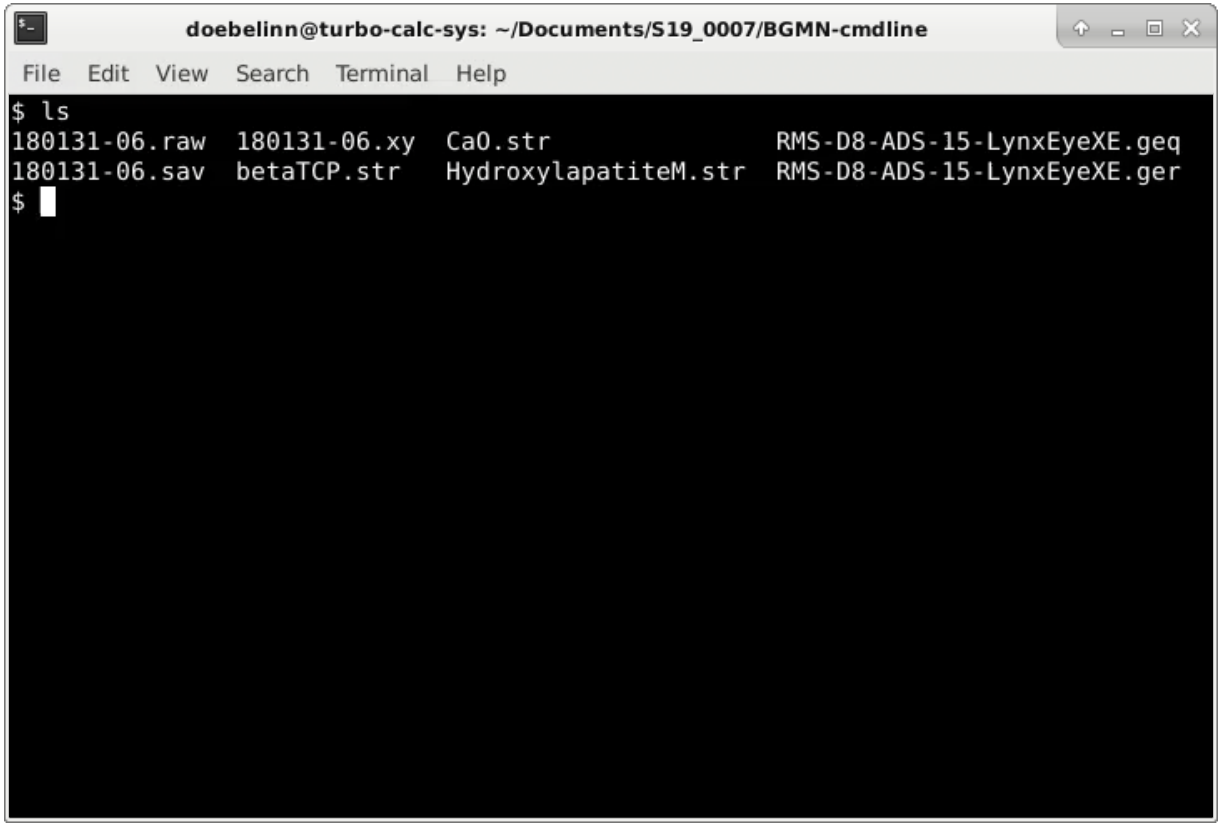
Nicola Döbelin

RMS Foundation, Bettlach, Switzerland

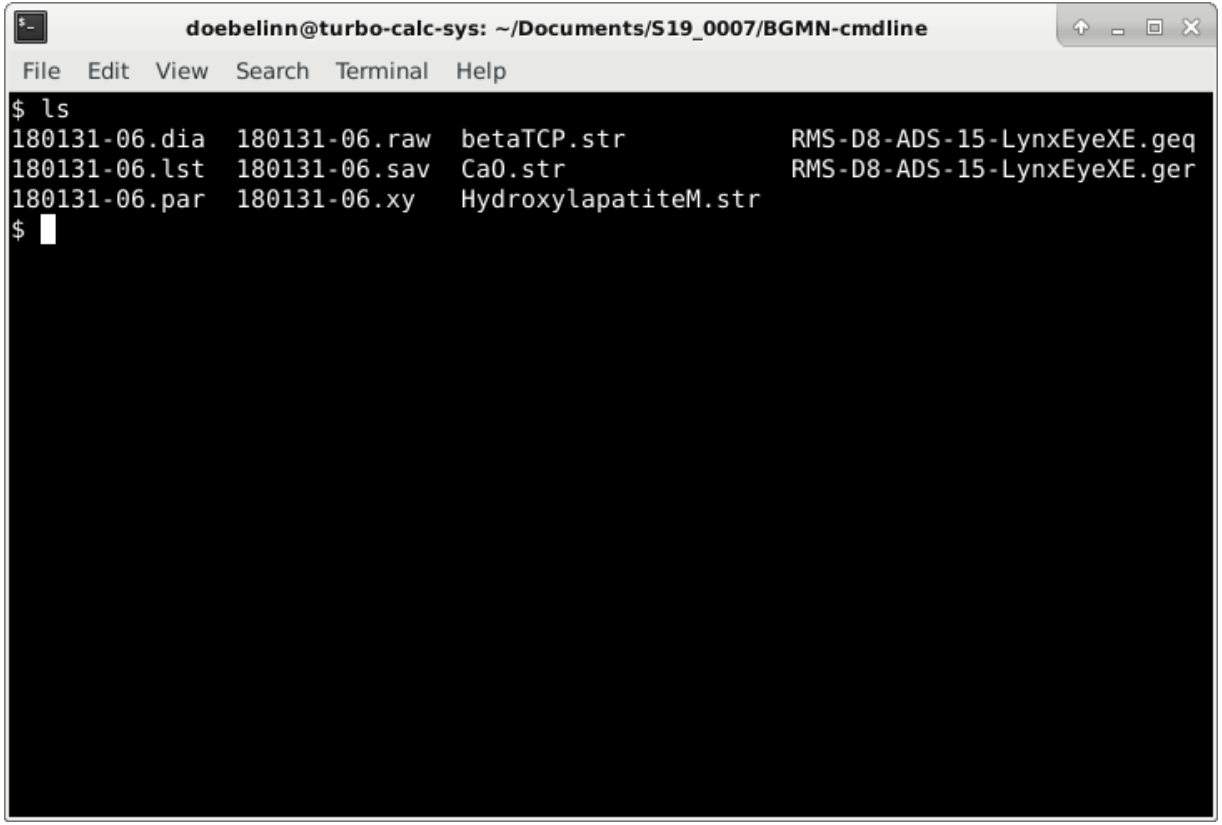
BGMN: Based on Text Files



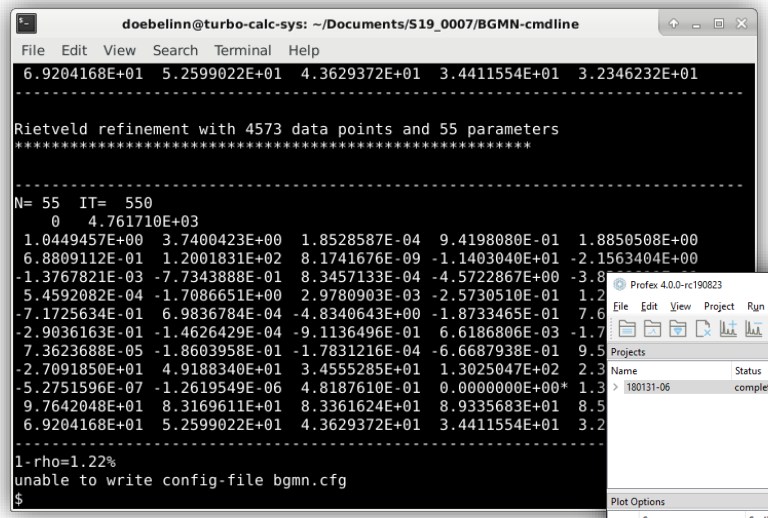
BGMN Command Line Application



BGMN Command Line Application

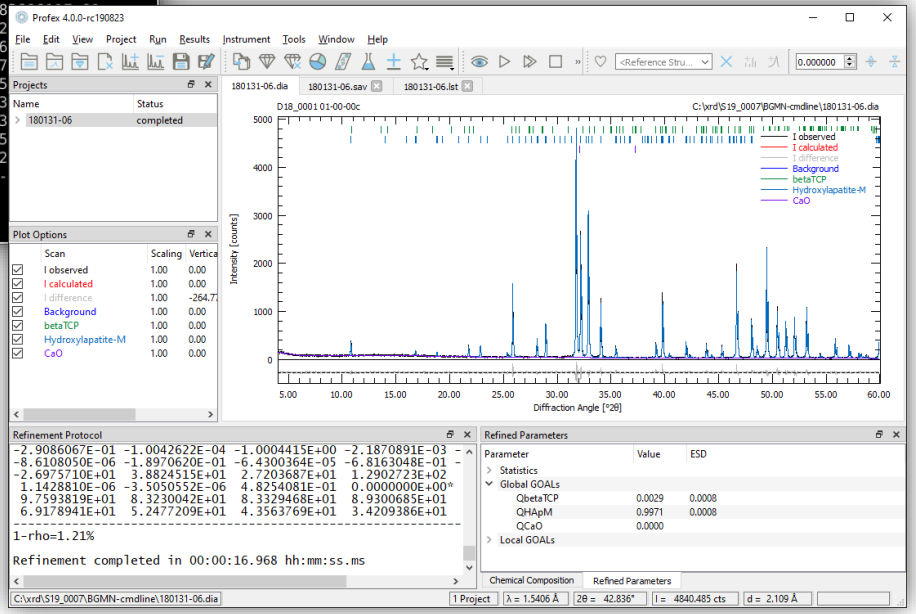


Graphical User Interfaces for BGMN



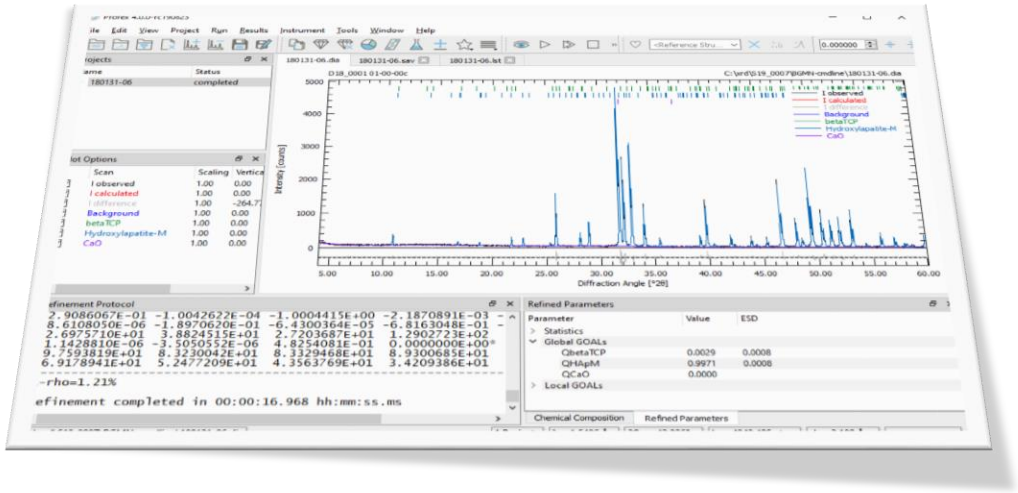
← BGMN can be used from a command shell. No user interface is required.

But much more convenient with a user interface →



Profex – A Graphical User Interface for BGMN

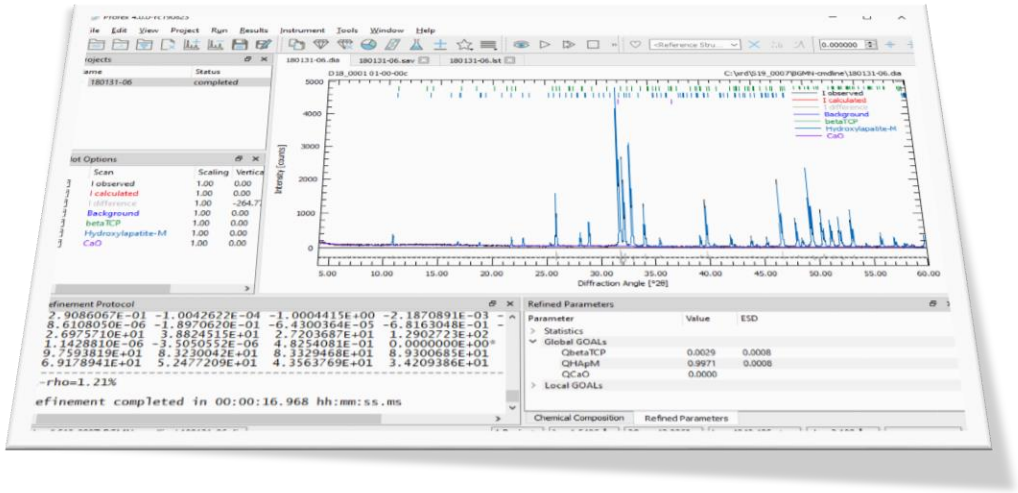
Developer:	Nicola Döbelin (private)
License:	GPL v2 or later (open source)
Founded in:	2003
Platforms:	Windows 7 / 8 / 8.1 / 10
	Mac OS X 10.9 -10.14 (64bit)
	Linux
Rietveld Backends:	BGMN, Fullprof.2k
Website:	http://www.profex-xrd.org
Current stable version:	4.0.0



Profex – A Graphical User Interface for BGMN

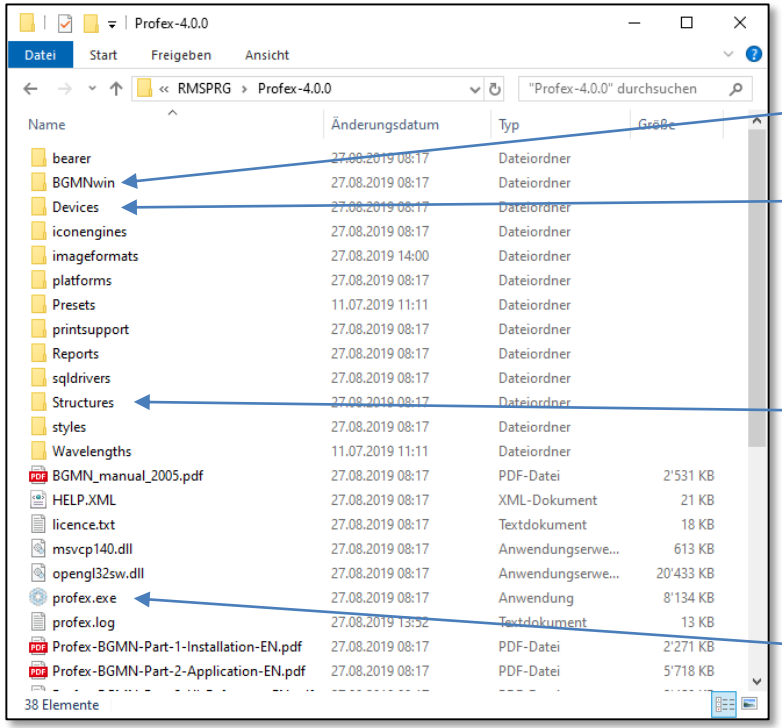
Version 4.0.0:

- Released in August 2019
- Bundled with BGMN
- Includes >750 structure files
  (~400 by BGMN team + ~350 by Profex)
- Includes 35 instrument configurations
- Many new features:
  - Search/Match
  - Electron density maps
  - Reporting
  - …



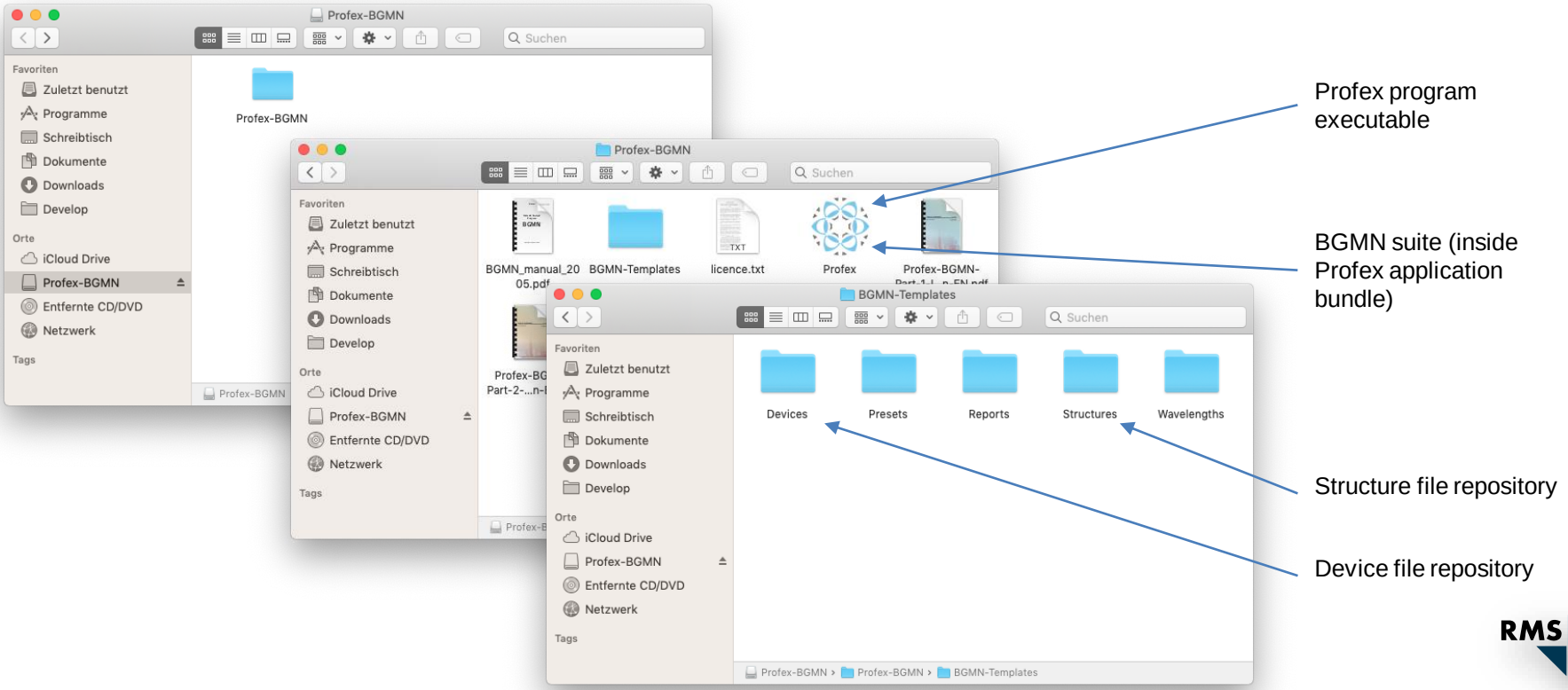
Installing Profex

- Windows: Installer (*.exe) or portable bundle (*.zip)
- OS X: Compressed disk image (*.dmg.zip)
- Linux: Source code



Installing Profex

- Windows: Installer (*.exe) or portable bundle (*.zip)
- OS X: Compressed disk image (*.dmg.zip)
- Linux: Source code

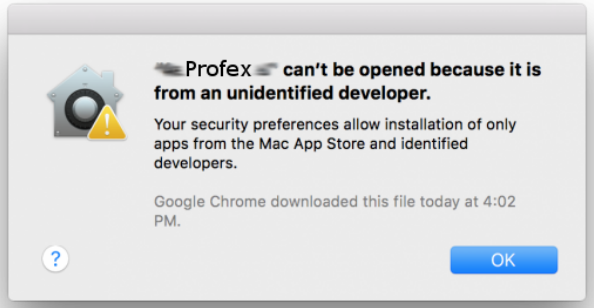


Profex: First Start Security Warnings

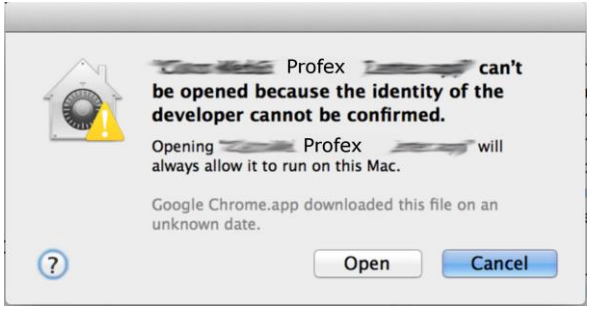
Windows

«More Info» → «Run anyway»

OS X:

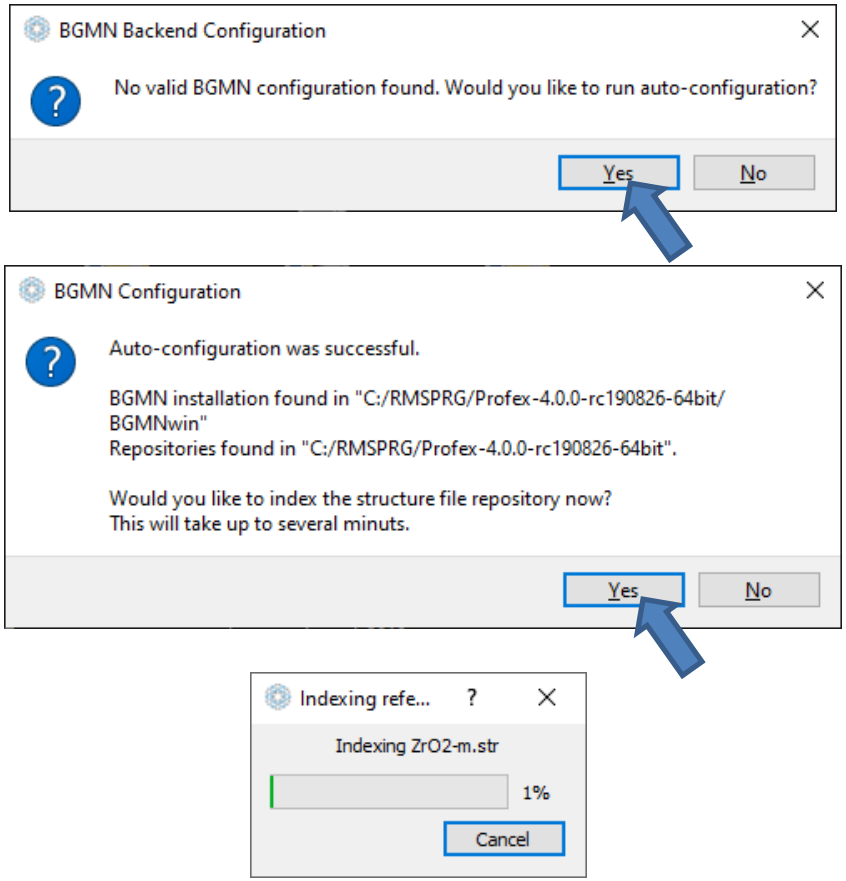


Ctrl + Click on Profex → "Open"

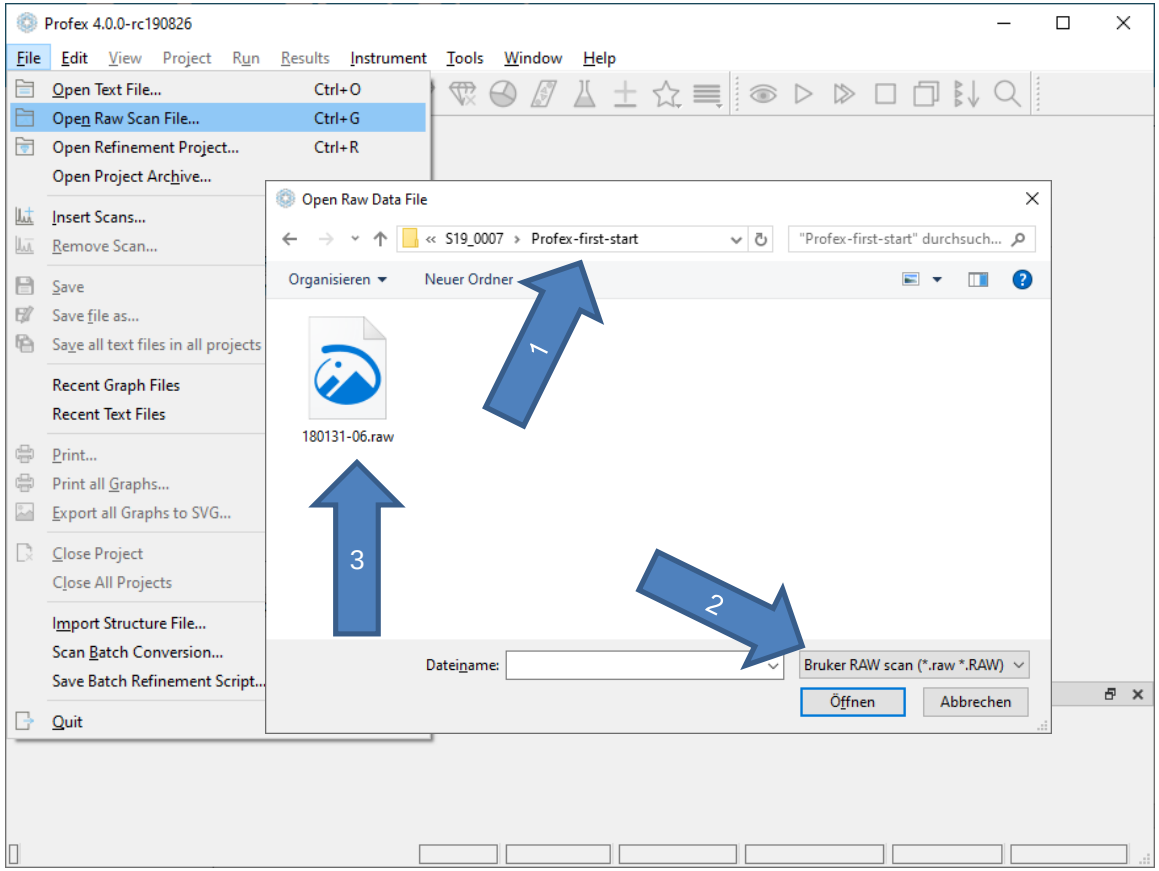


«Open»

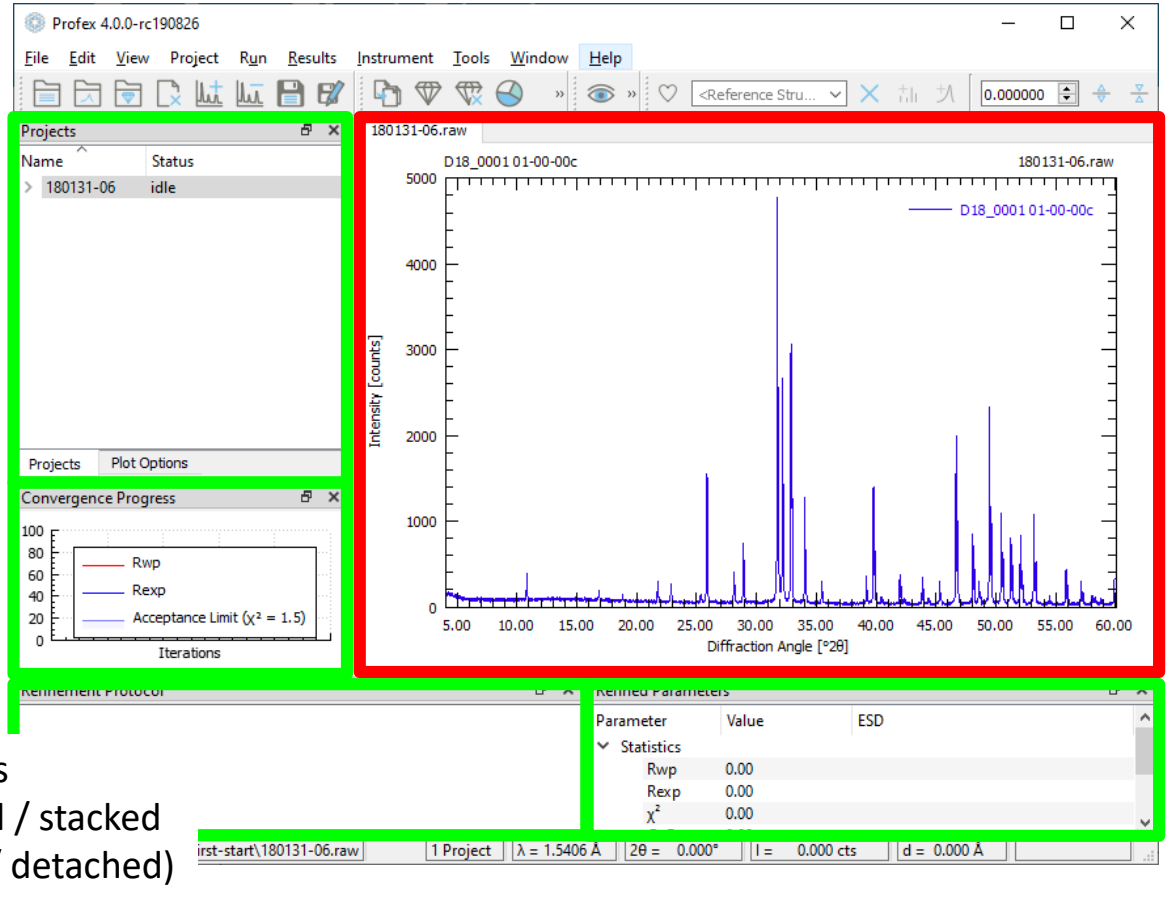
Profex: First Start



Profex: First Start



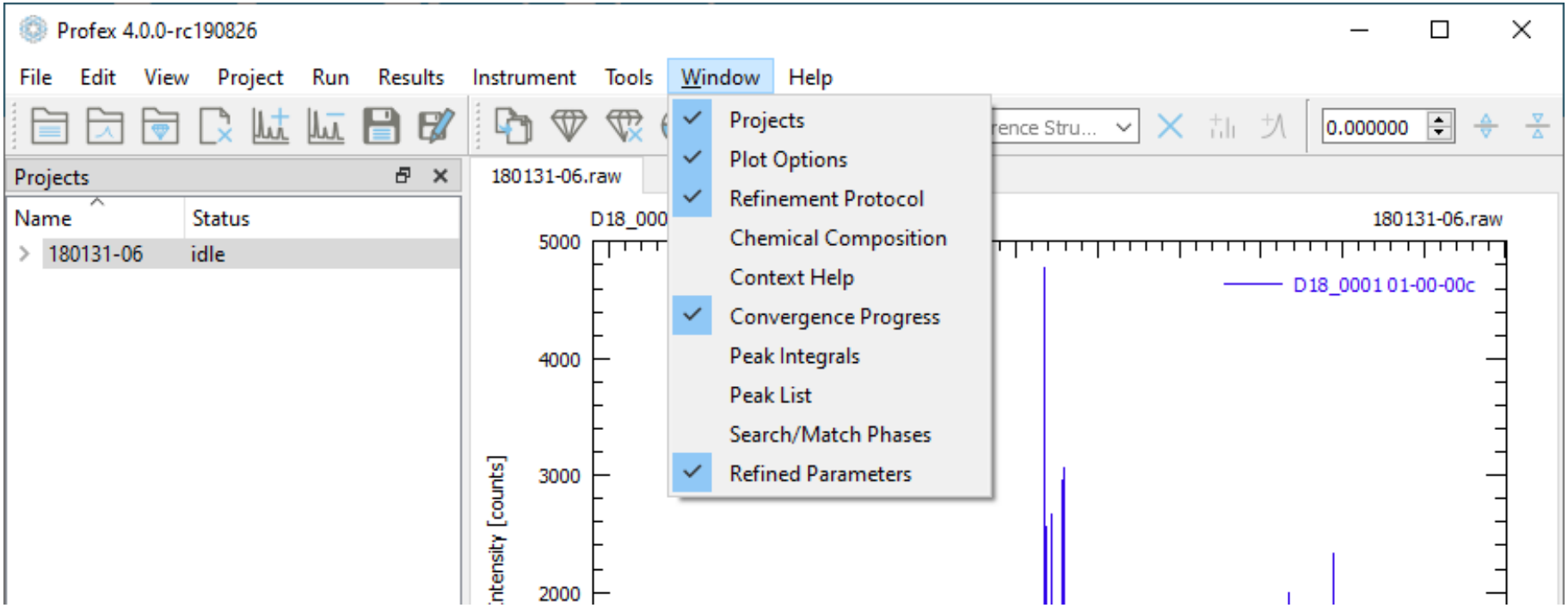
Profex: First Start



Plot area
(cannot be closed)

Dock windows
(can be closed / stacked
/ rearranged / detached)

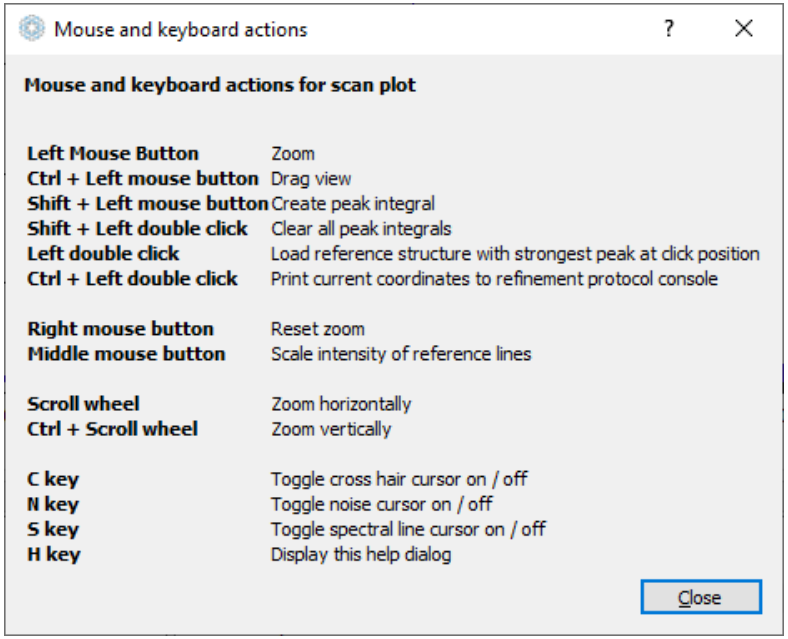
Profex: First Start



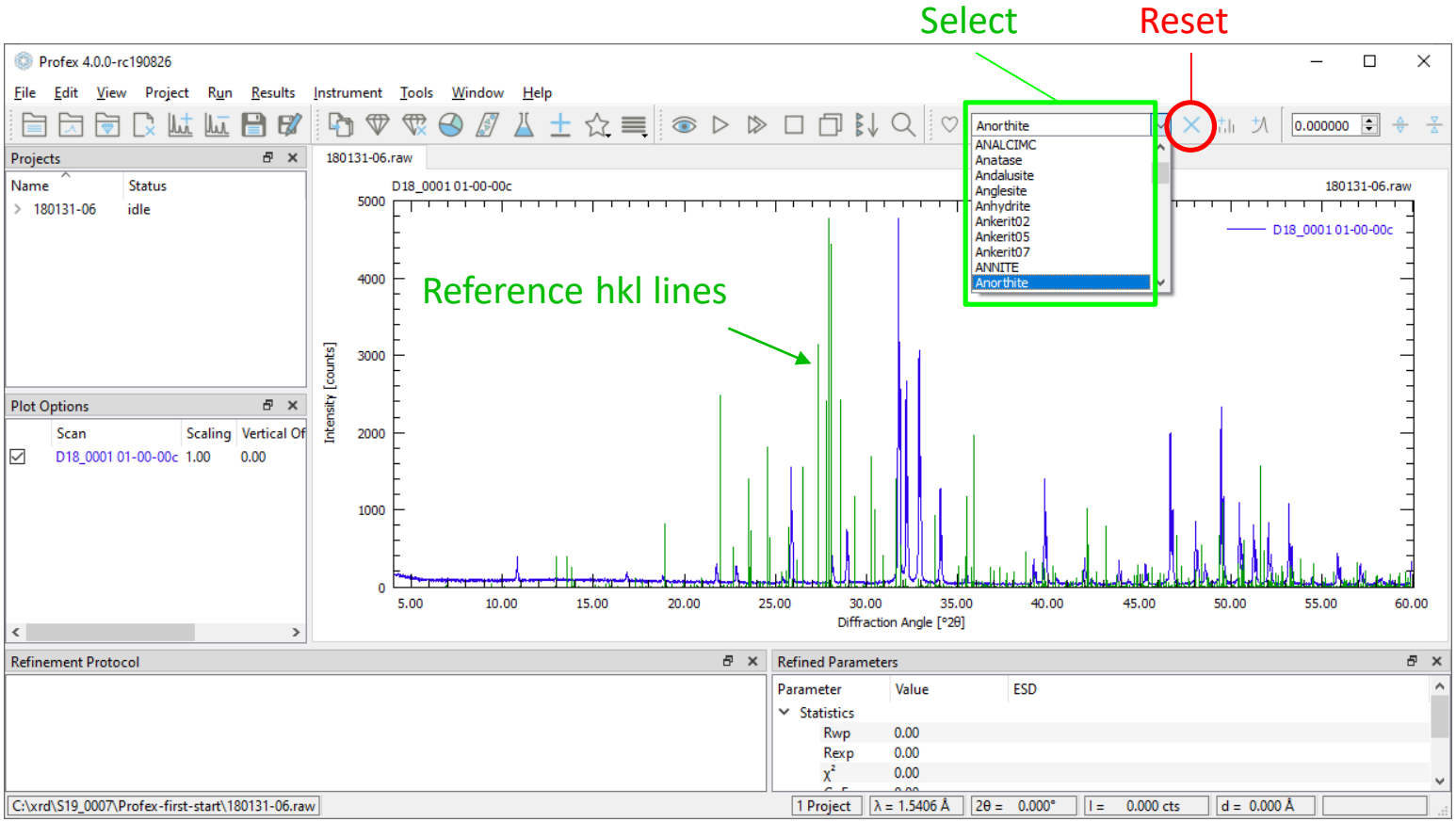
Closed Dock Windows can be re-opened
from the «Window» menu

Profex: First Start

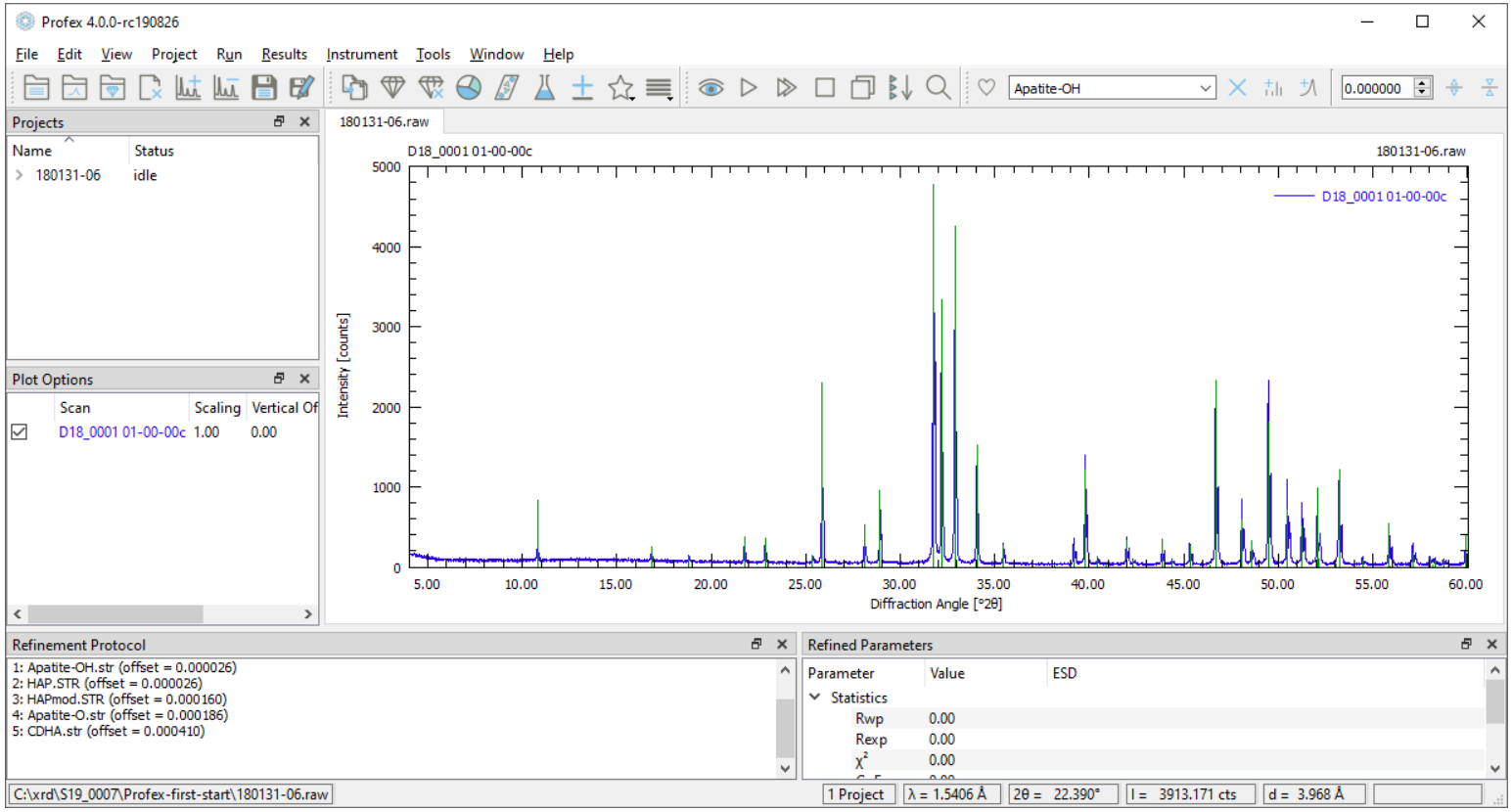
Help → Mouse and Keyboard Commands:



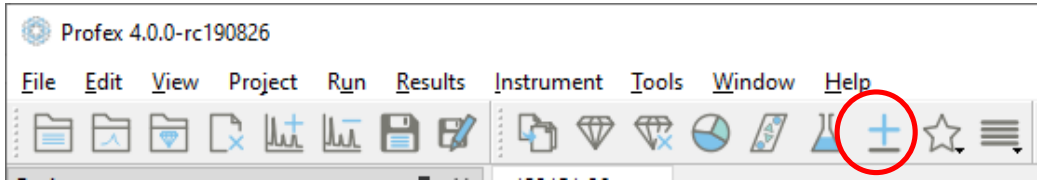
Indexed Reference Structures

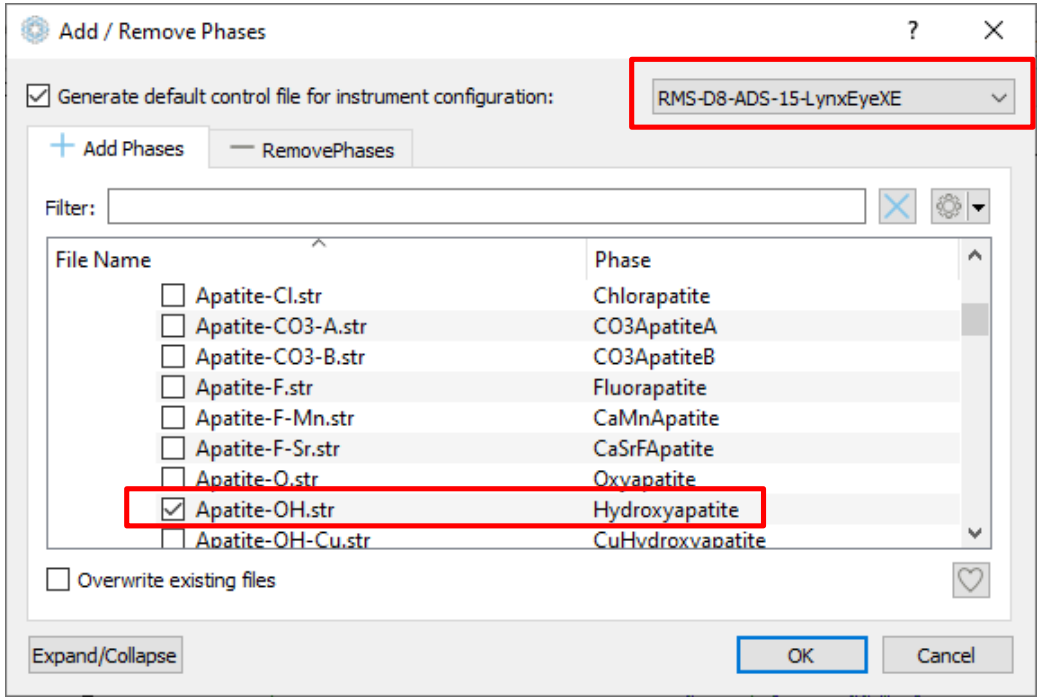


Step 1: Identify Phases



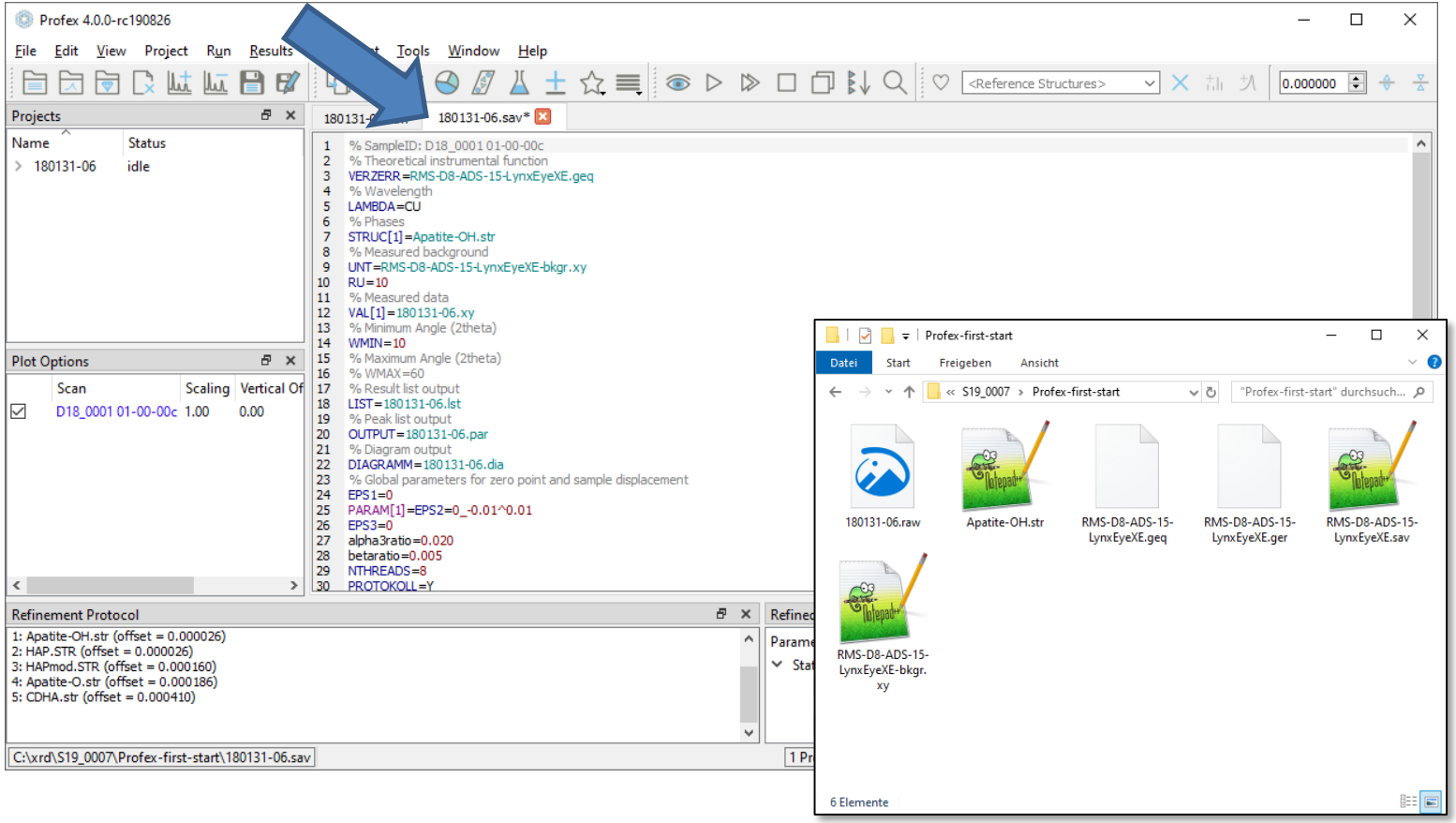
Step 2: Create Refinement Project





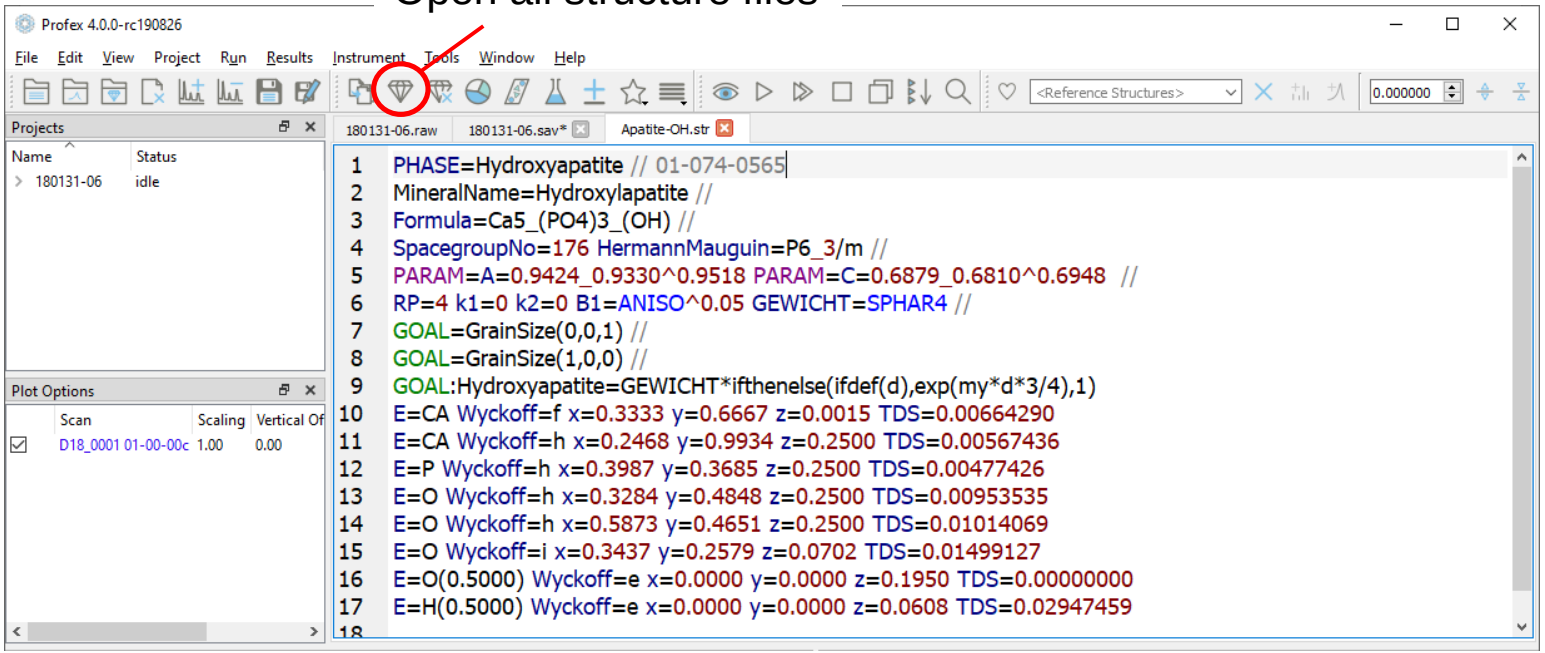
1. Click «Add/Remove Phase»
2. Select correct instrument configuration
3. Select identified phases
4. Click «OK»

Step 2: Create Refinement Project



Step 3: Release parameters for refinement

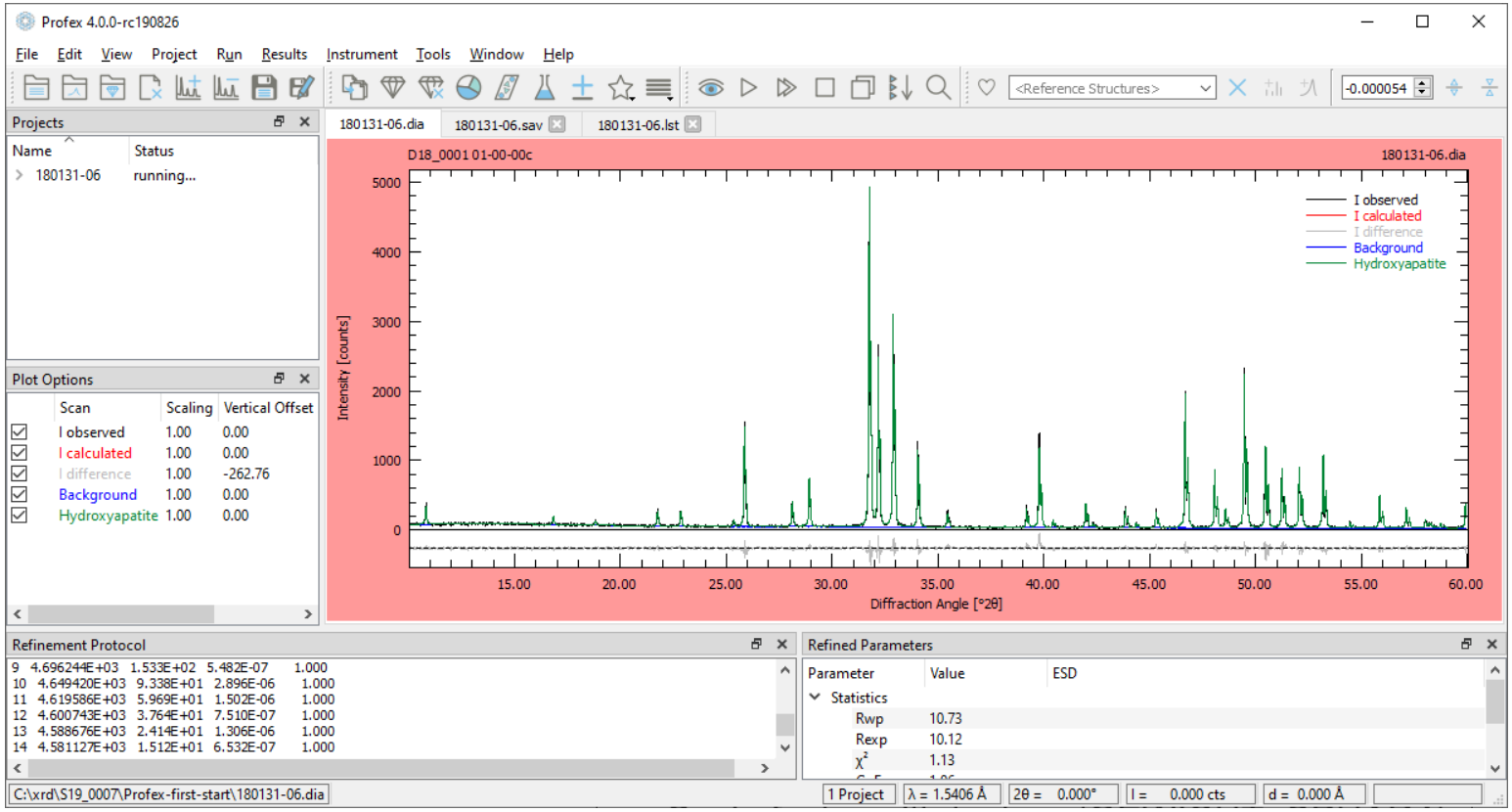
Open all structure files



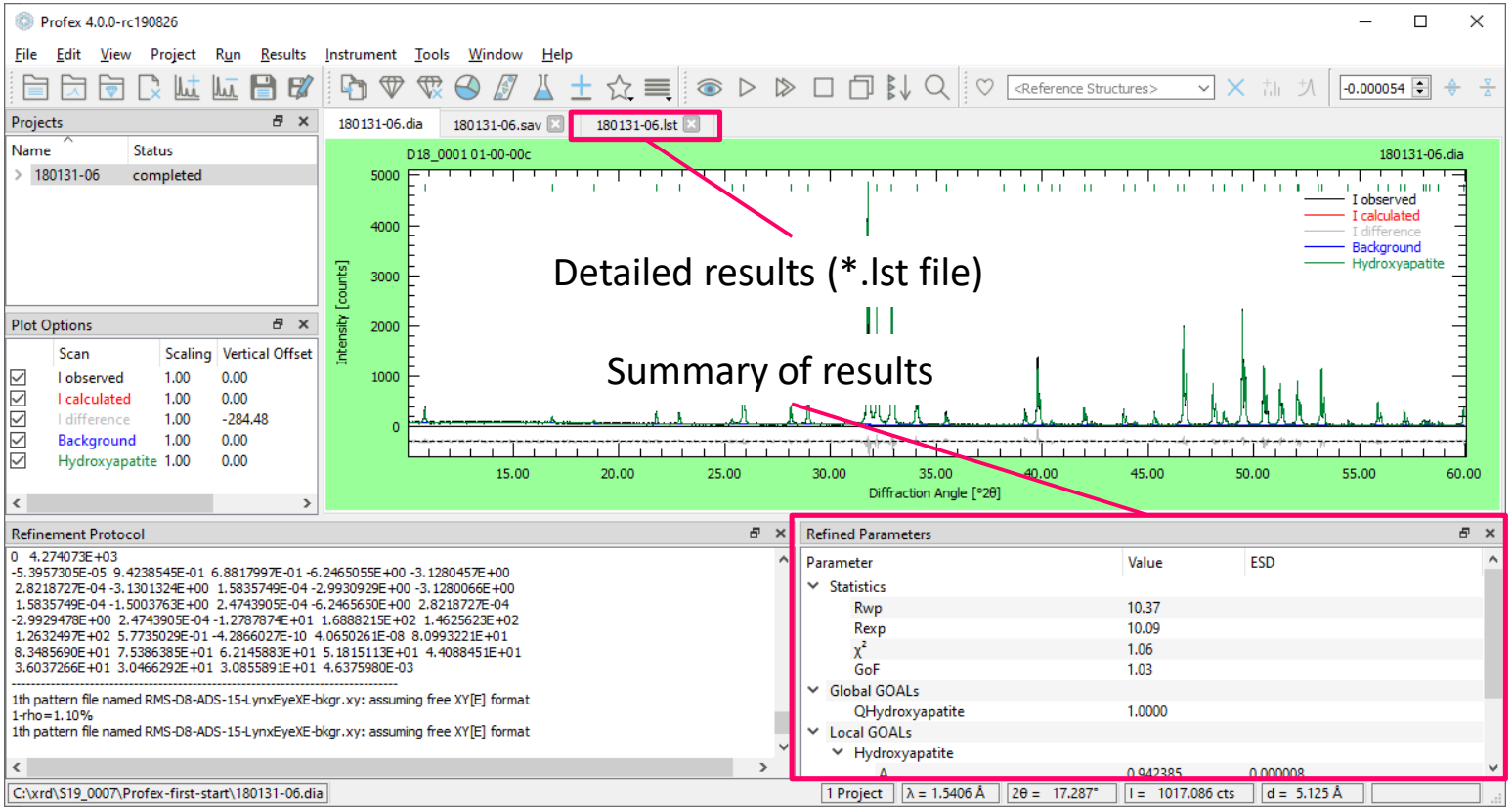
Already released for refinement:

- Unit cell A and C
- Crystallite size (B1)
- Scale factor with texture (GEWICHT=SPHAR4)

Step 4: Run the refinement

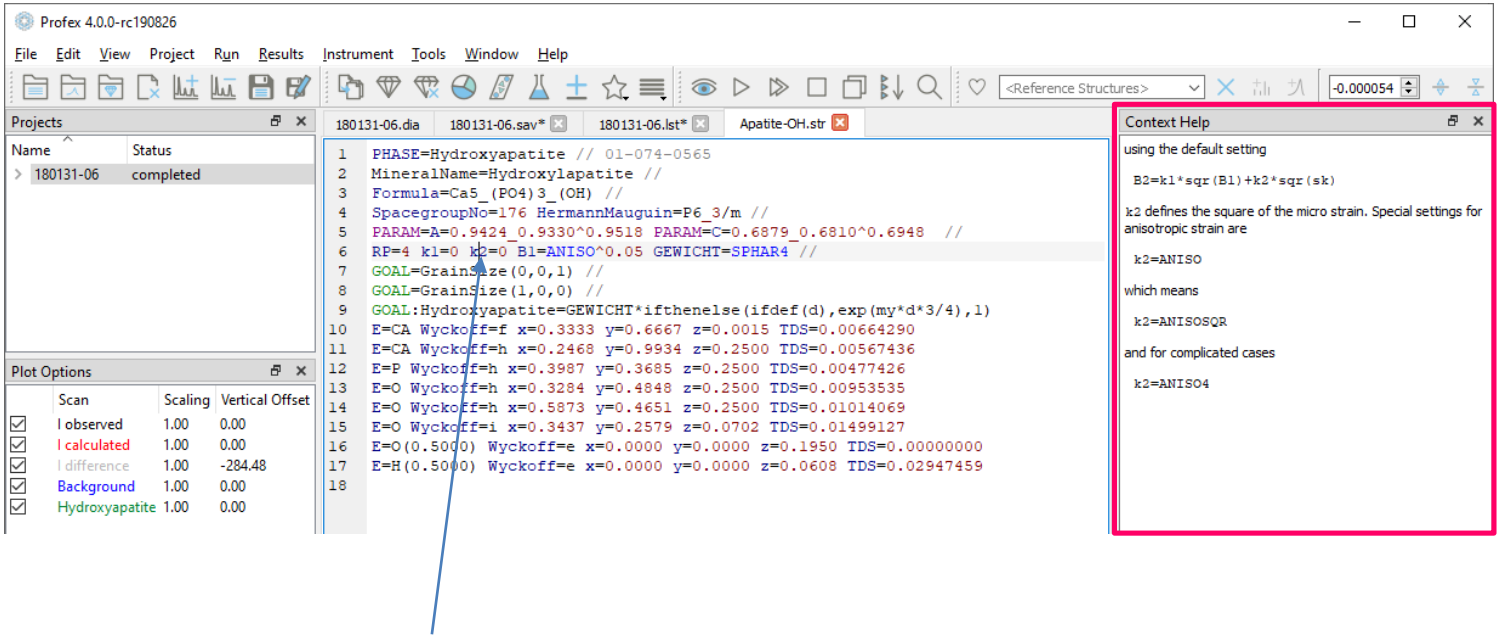


Results


Profex 4.0.0-rc190826
File Edit View Project Run Results Instrument Tools Window Help
Projects
Name Status
180131-06 completed
Plot Options
Scan Scaling Vertical Offset
I observed 1.00 0.00
I calculated 1.00 0.00
I difference 1.00 -284.48
Background 1.00 0.00
Hydroxyapatite 1.00 0.00
180131-06.dia
180131-06.sav
180131-06.lst
D18_0001 01-00-00c
180131-06.dia
I observed
I calculated
I difference
Background
Hydroxyapatite
Intensity [counts]
Diffraction Angle [°2θ]
Detailed results (*.lst file)
Summary of results
Refinement Protocol
Refined Parameters
Parameter Value ESD
Statistics
Rwp 10.37
Rexp 10.09
χ² 1.06
GoF 1.03
Global GOALs
QHydroxyapatite 1.0000
Local GOALs
Hydroxyapatite
C:\xrd\S19_0007\Profex-first-start\180131-06.dia
1 Project
λ = 1.5406 Å
2θ = 17.287°
I = 1017.086 cts
d = 5.125 Å

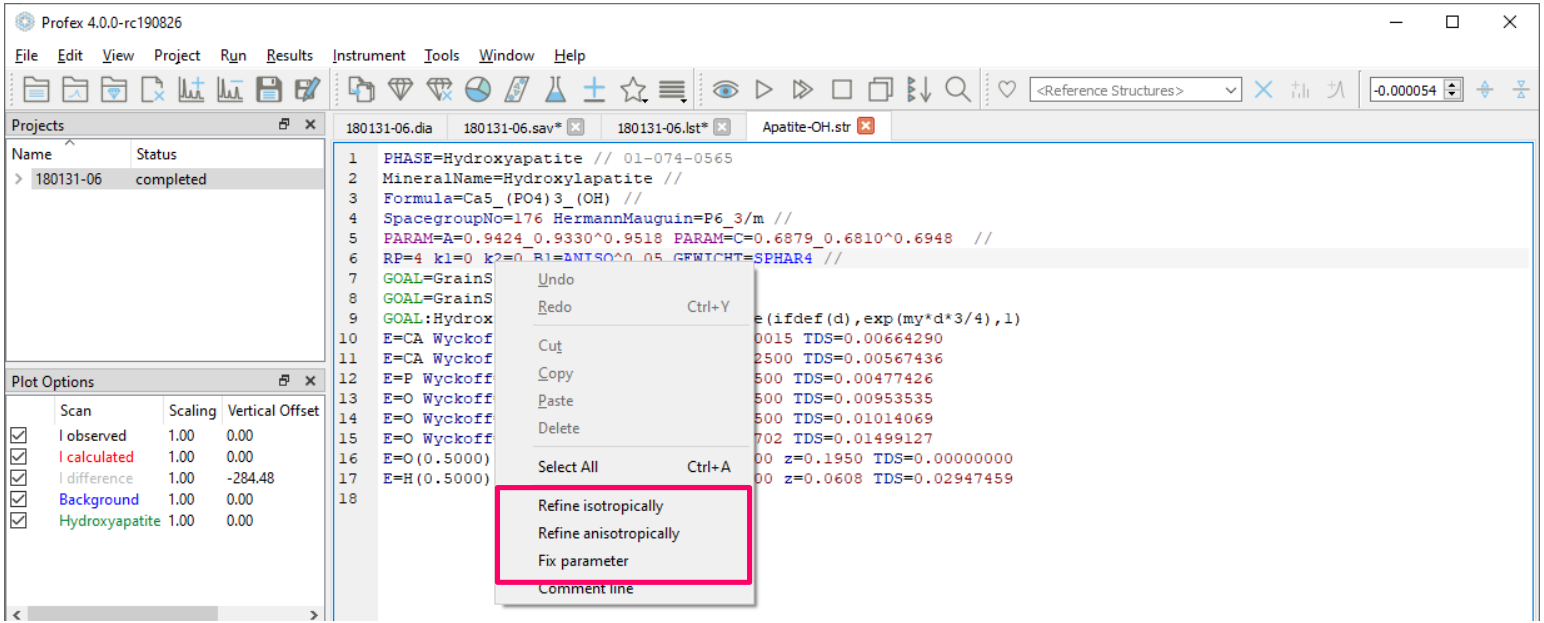
Context Help

Open «Window → Context Help»



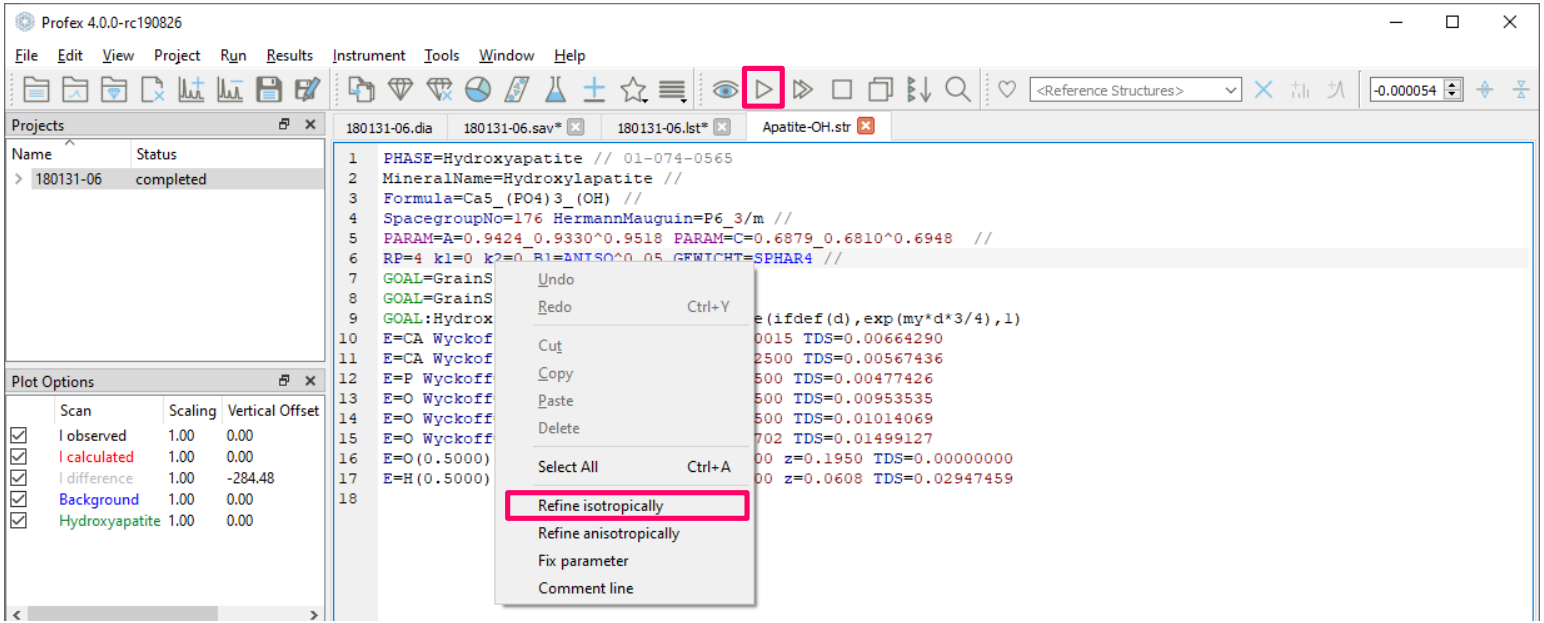
1. Place the cursor on a parameter (here: k2)
2. Press «F1» key

Release Micro-Strain for refinement



1. Open the Apatite-OH.str file (button)
2. Place the cursor on the parameter «k2»
3. Right mouse button to open context menu

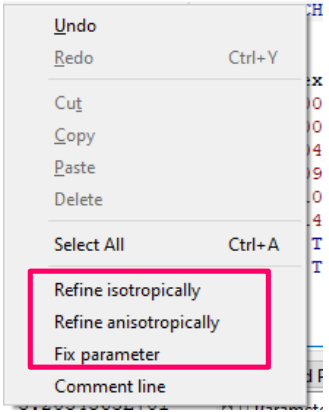
Release Micro-Strain for refinement



1. Select «Refine isotropically»
2. Run the refinement

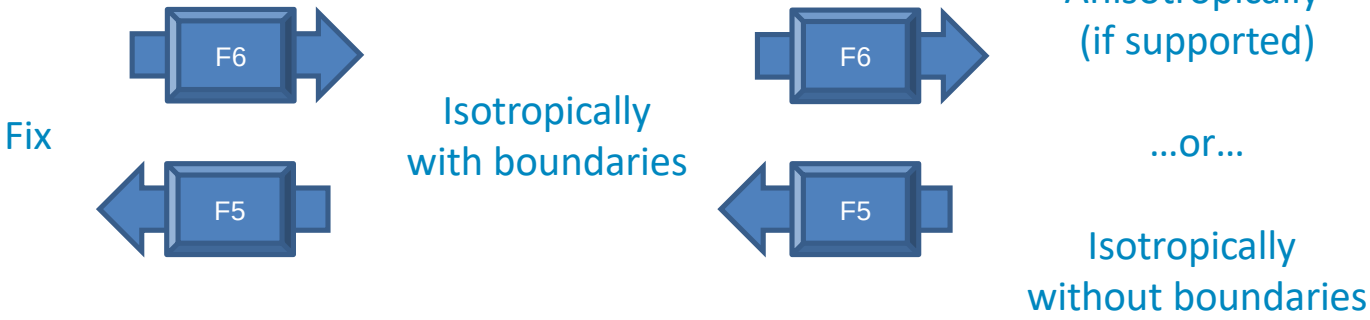
Releasing / Fixing Parameters for Refinement

1. Place cursor on parameter
2. Right mouse button
3. Select status from menu

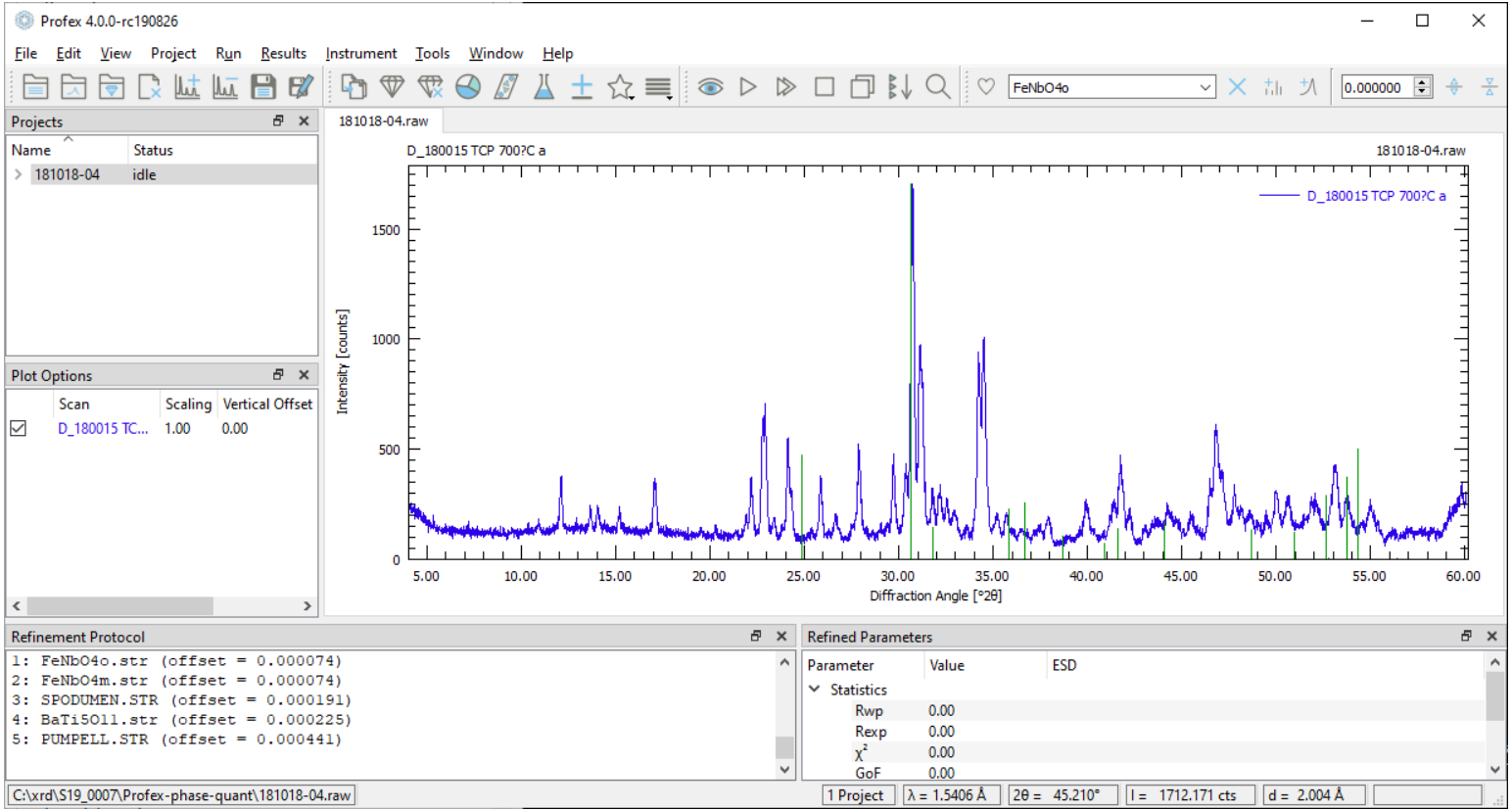


Alternatively:

1. Place cursor on parameter
2. Use «F5» and «F6» keys to change refinement status



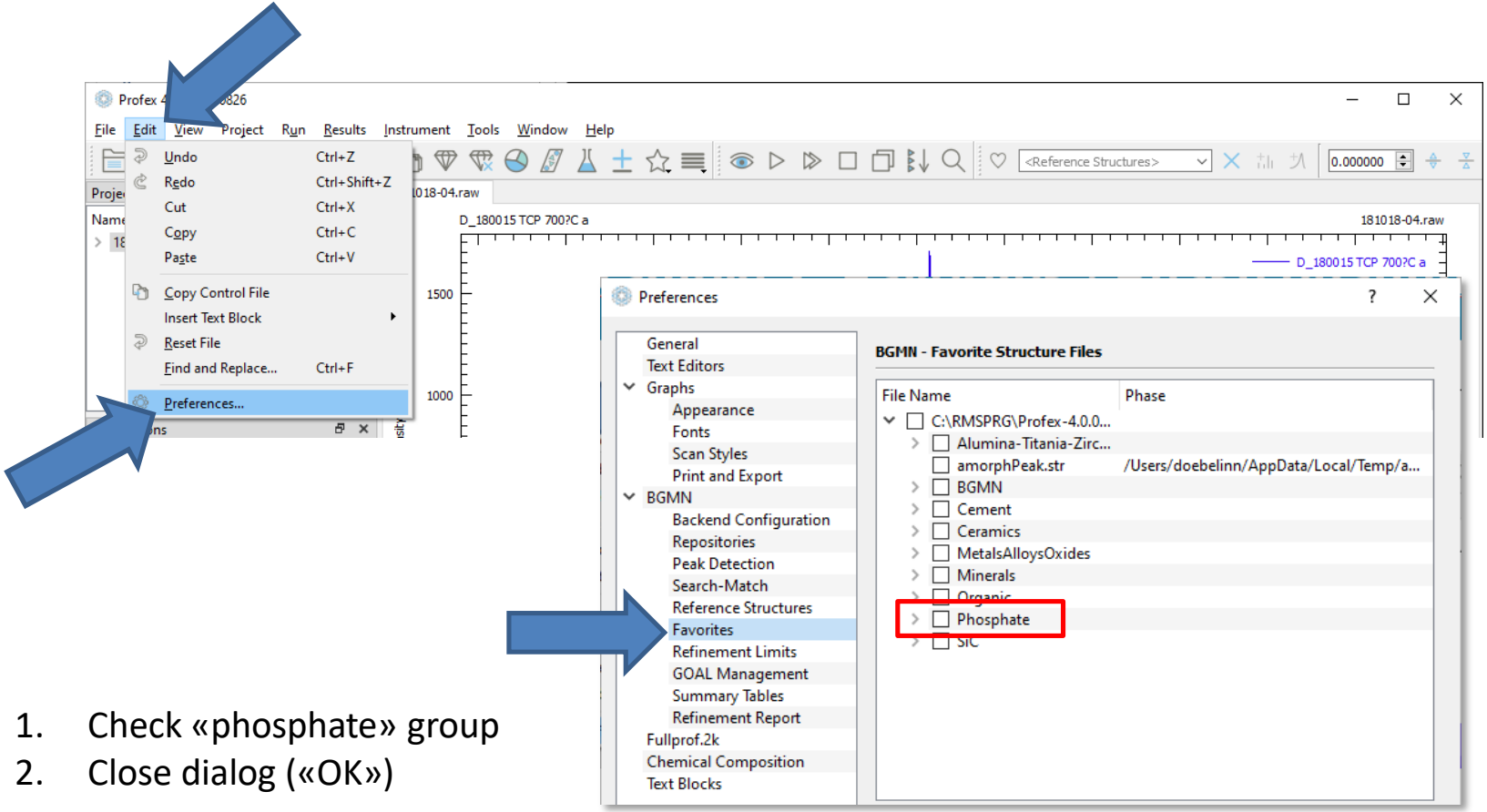
Example 2: Favorites / Phase quantification



Problems:

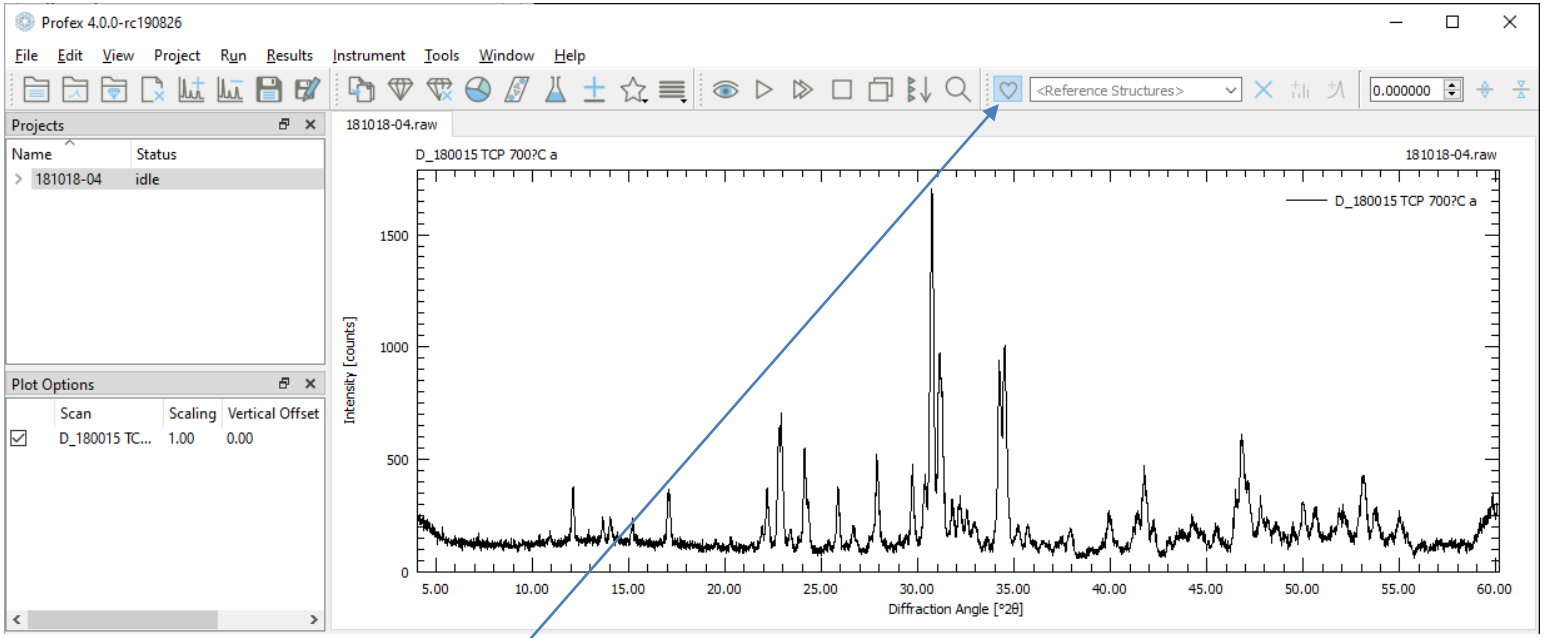
- Too many phases to chose from
- Highest intensity ≠ strongest peak (highest integrated intensity)

Example 2: Favorites / Phase quantification



1. Check «phosphate» group
2. Close dialog («OK»)

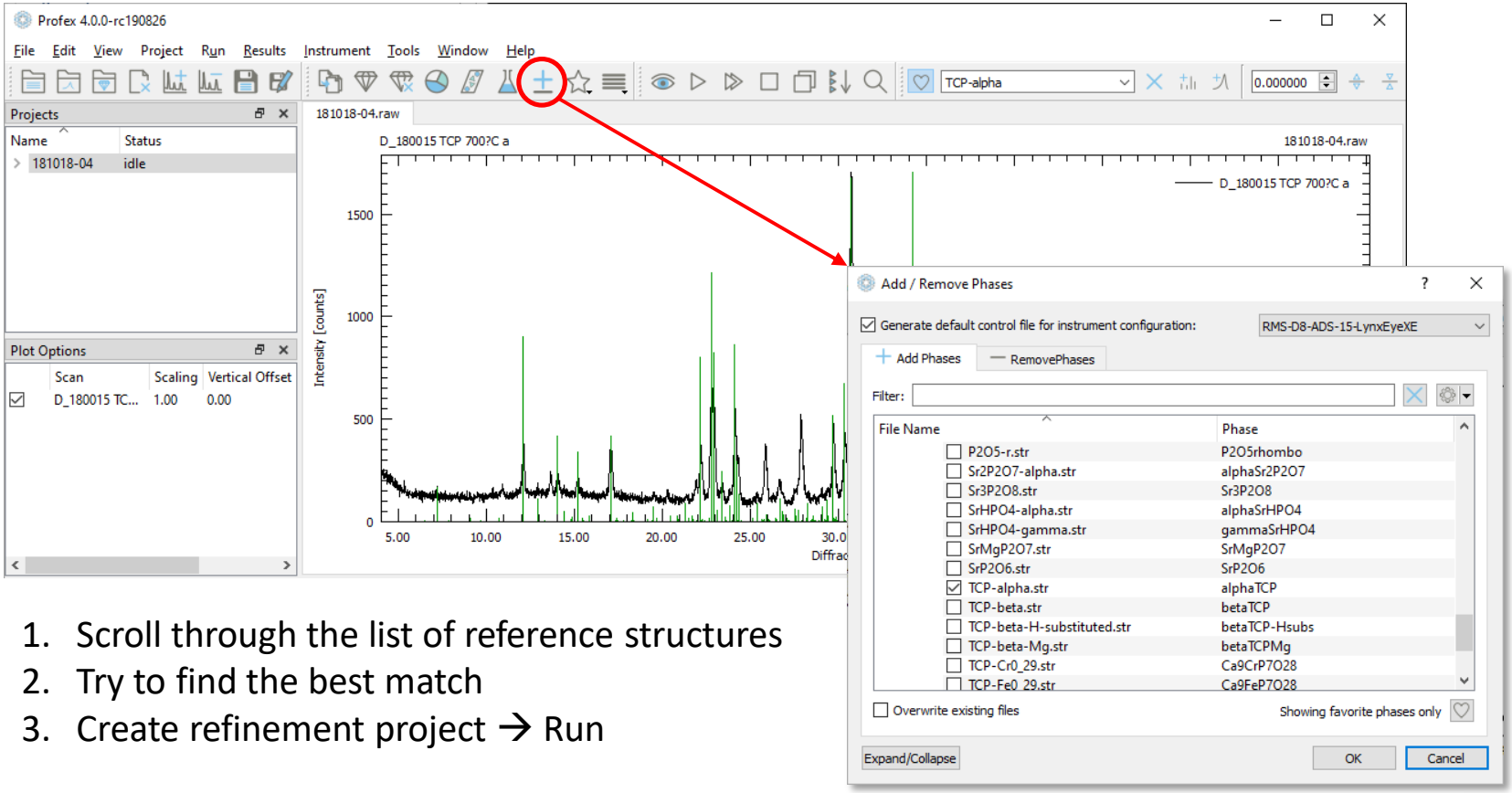
Example 2: Favorites / Phase quantification



«Favorites» button:

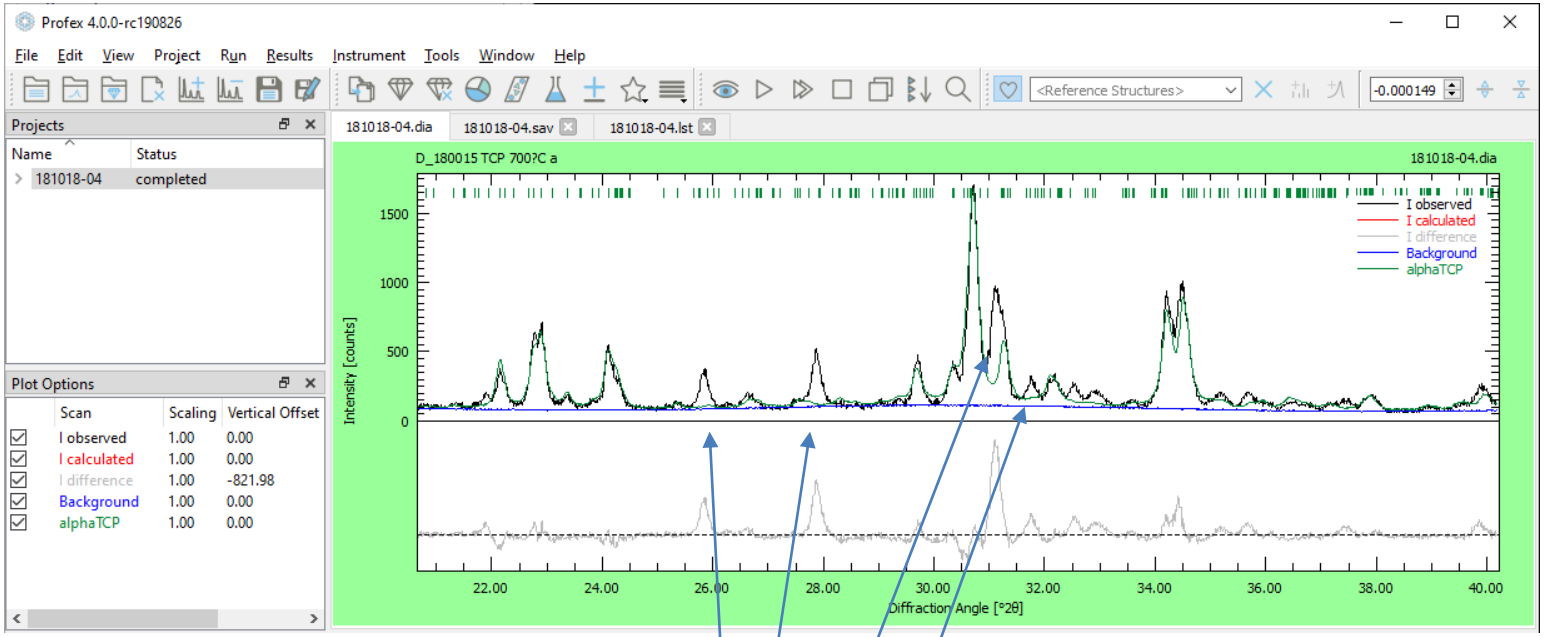
Check to limit the database to favorite phases only.
Double-clicking peaks only searches among favorite phases.

Example 2: Favorites / Phase quantification



1. Scroll through the list of reference structures
2. Try to find the best match
3. Create refinement project → Run

Example 2: Favorites / Phase quantification



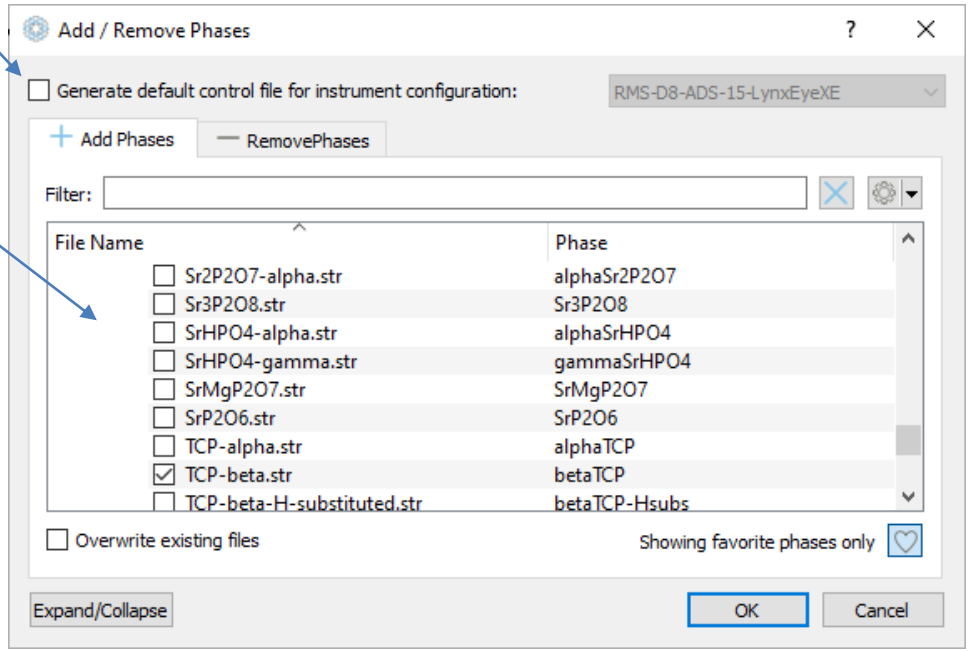
More unidentified phases

Use double-click or scroll through the reference structures to identify them.

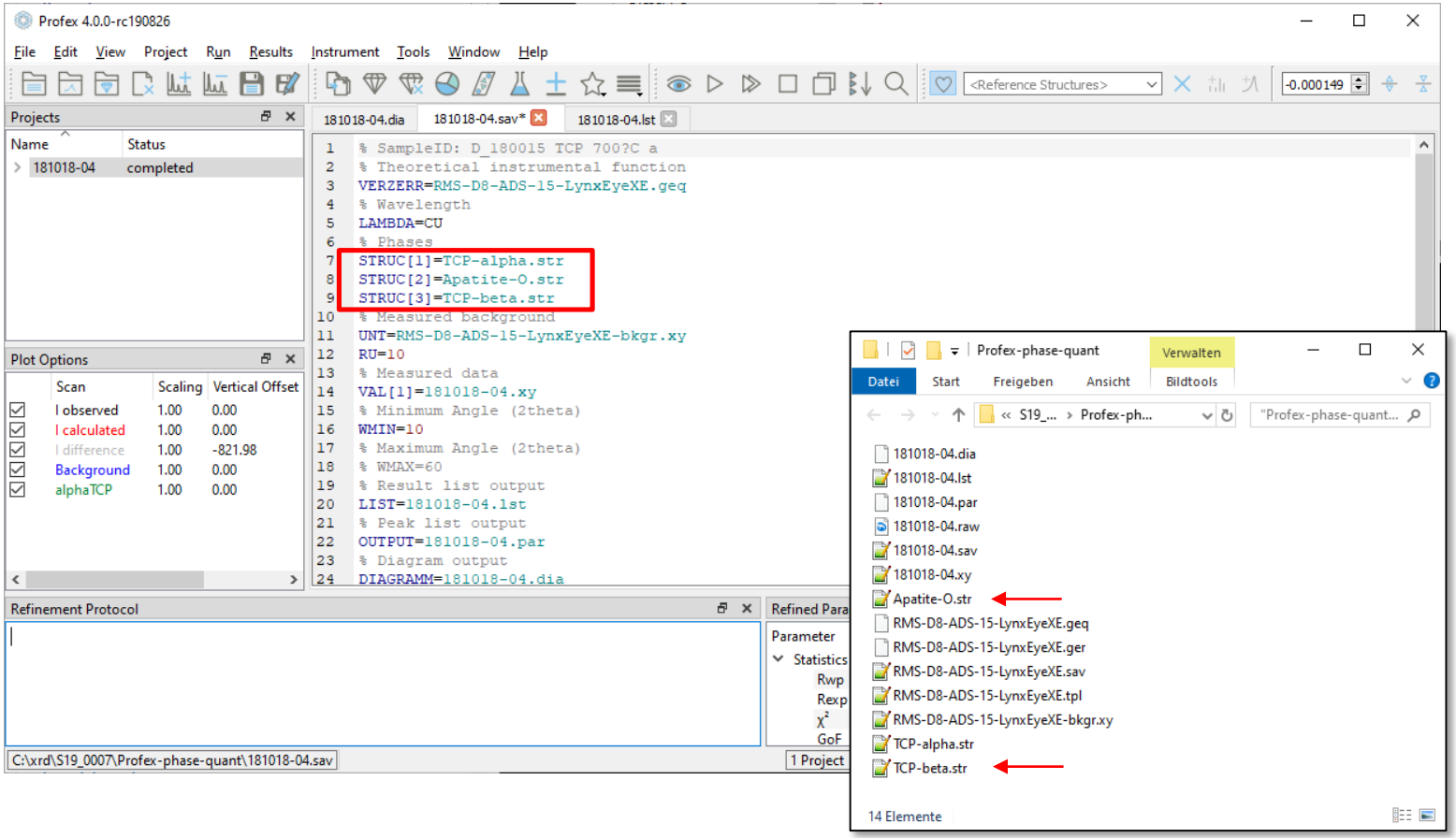
Example 2: Favorites / Phase quantification

1. Add/Remove phase: 
2. Leave this unchecked (we already have a control file)

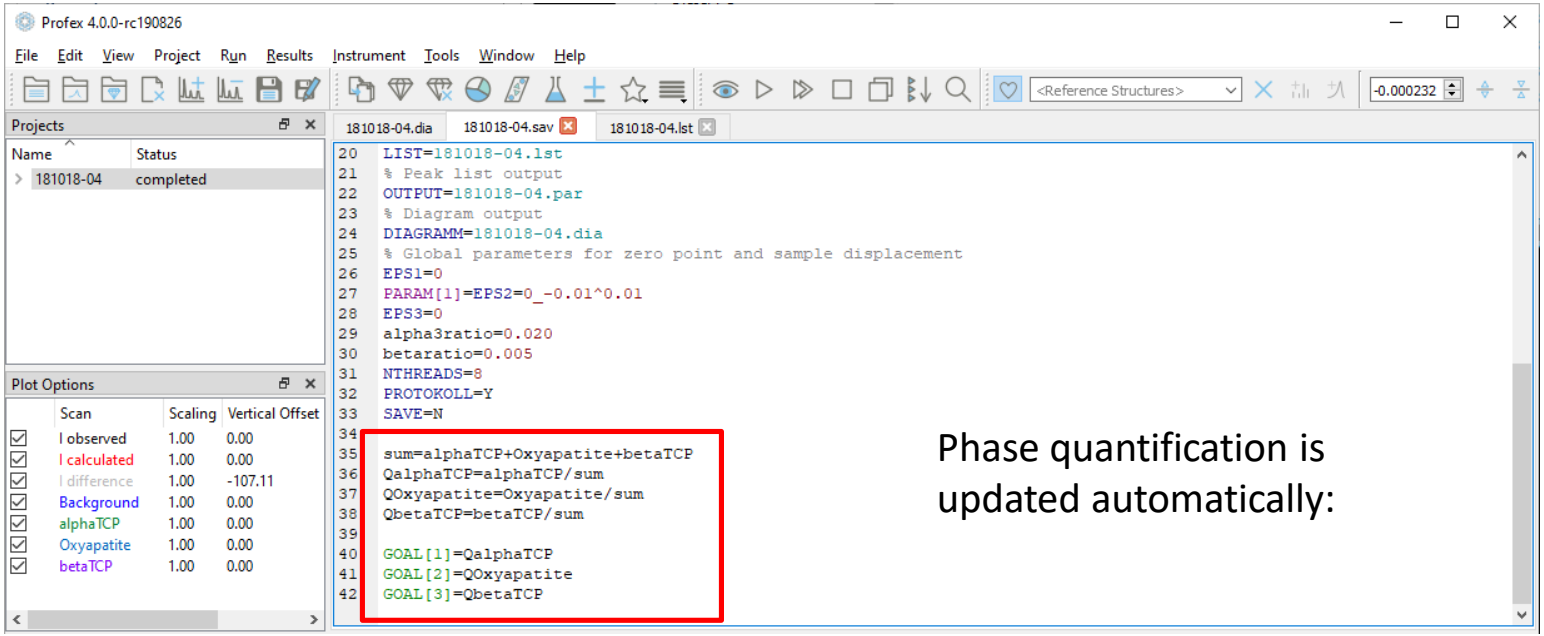
3. Select identified phases
4. → «OK»



Example 2: Favorites / Phase quantification



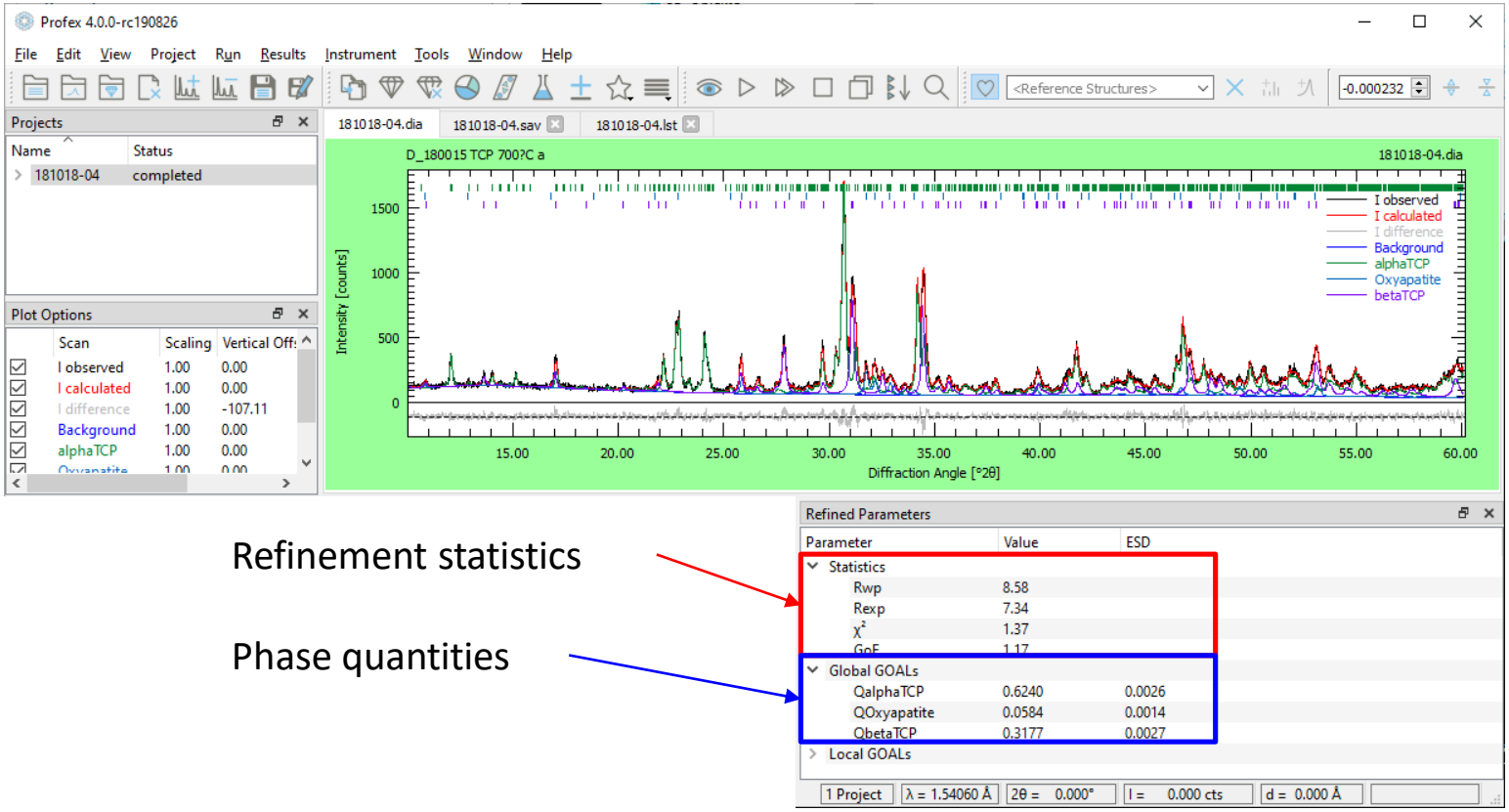
Example 2: Favorites / Phase quantification



Phase quantification is updated automatically:

$$sum = \sum GEWICHT \qquad Q_{Phase} = \frac{GEWICHT_{Phase}}{sum}$$

Example 2: Favorites / Phase quantification

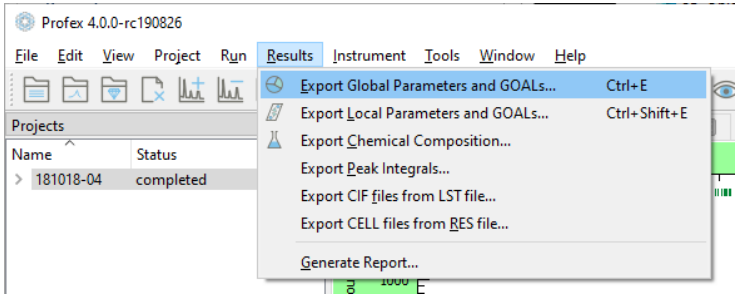


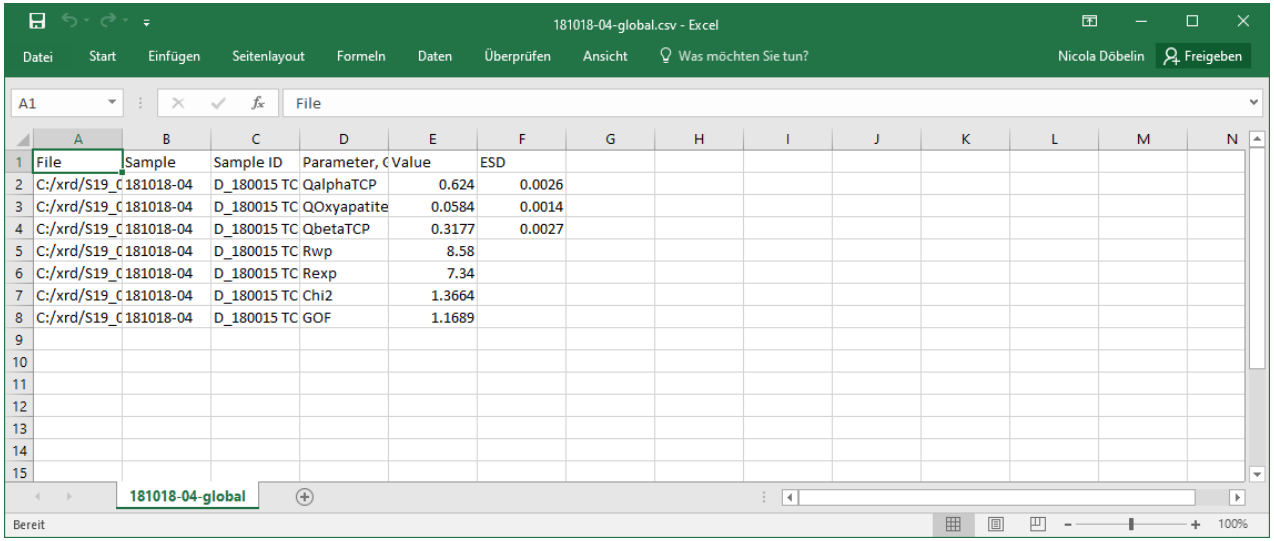
Refinement statistics

Phase quantities

If necessary: Release / fix parameters in STR files → Repeat refinement

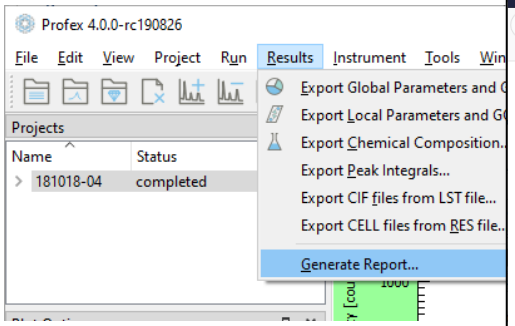
Example 2: Exporting Results

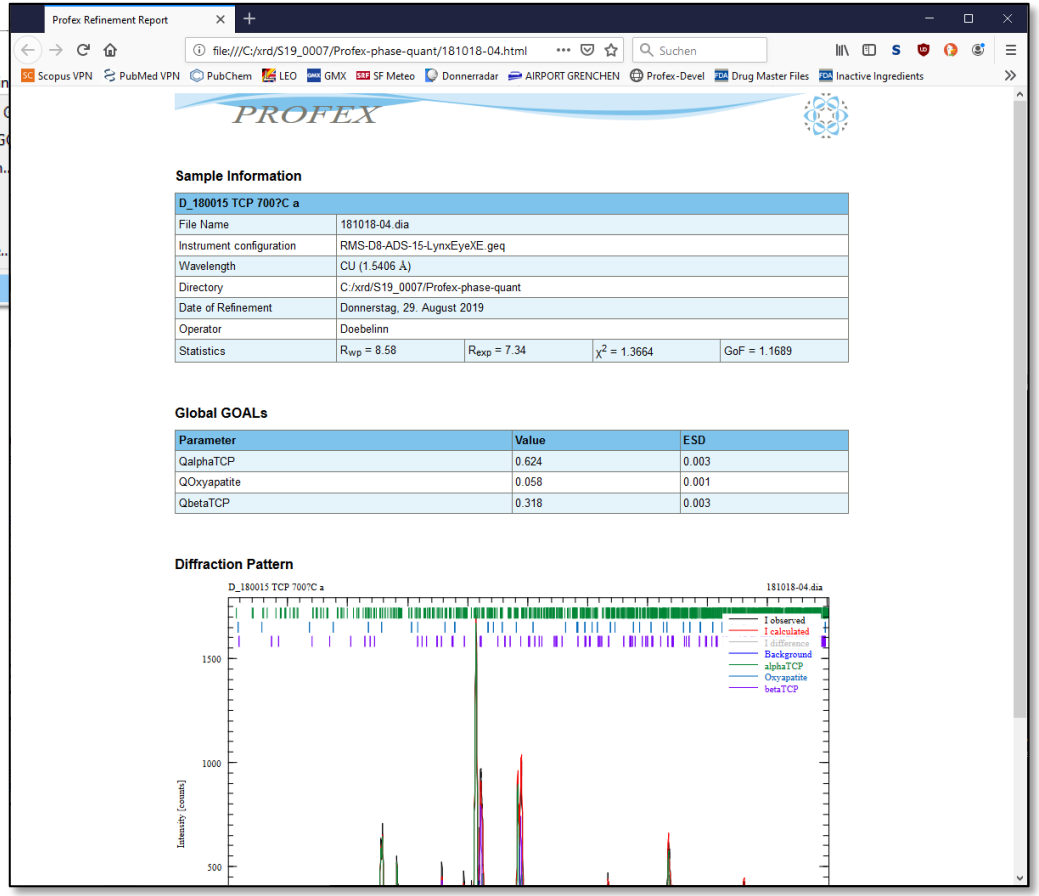




	File	Sample	Sample ID	Parameter, C	Value	ESD
2	C:/xrd/S19_C	181018-04	D_180015 TC	QalphaTCP	0.624	0.0026
3	C:/xrd/S19_C	181018-04	D_180015 TC	QOxyapatite	0.0584	0.0014
4	C:/xrd/S19_C	181018-04	D_180015 TC	QbetaTCP	0.3177	0.0027
5	C:/xrd/S19_C	181018-04	D_180015 TC	Rwp	8.58	
6	C:/xrd/S19_C	181018-04	D_180015 TC	Rexp	7.34	
7	C:/xrd/S19_C	181018-04	D_180015 TC	Chi2	1.3664	
8	C:/xrd/S19_C	181018-04	D_180015 TC	GOF	1.1689	

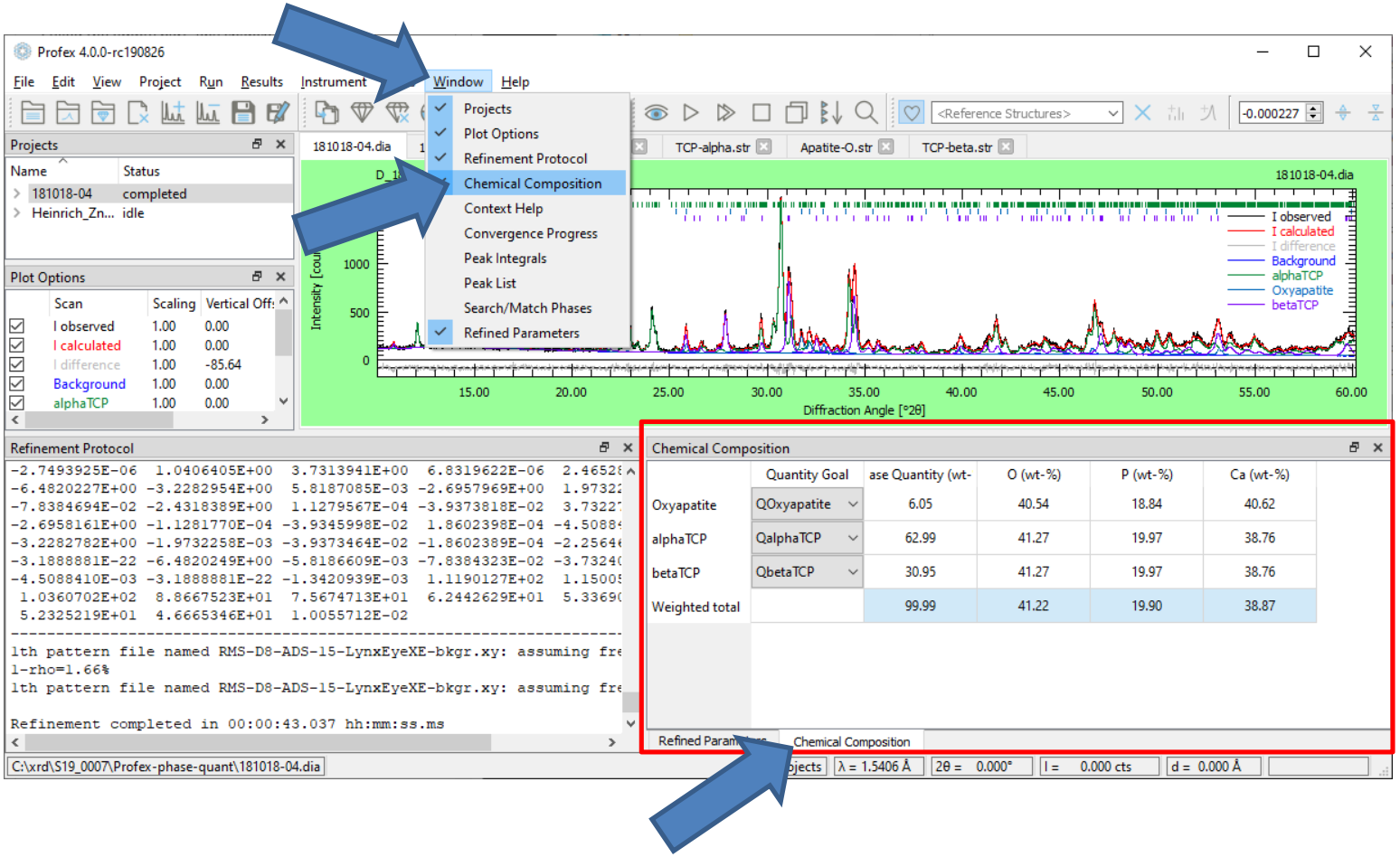
Example 2: Exporting Results





Report in HTML format
(opens in web browser)

Example 2: Refined Chemical Composition



Example 2: Refined Chemical Composition

Chemical Composition

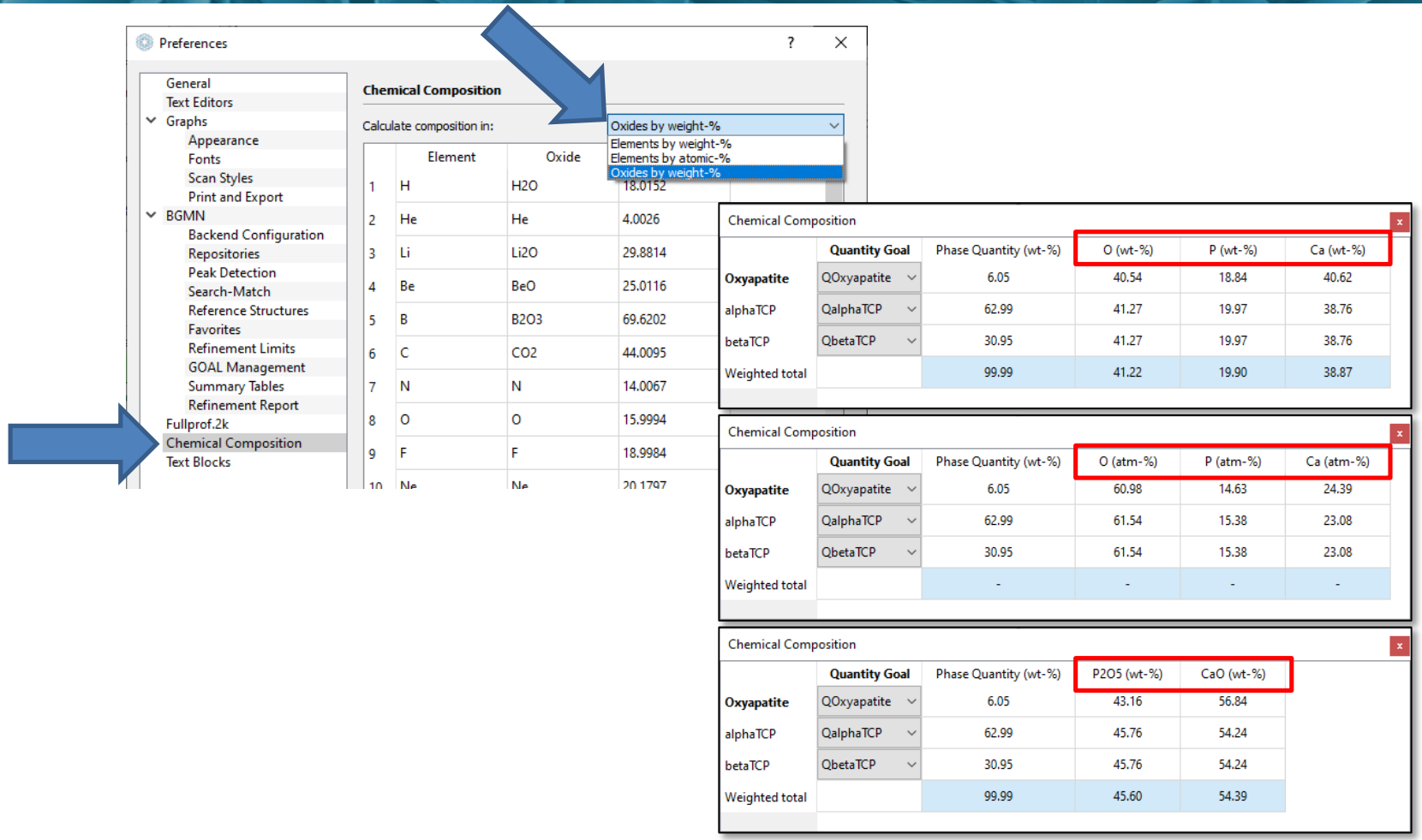
	Quantity Goal	Phase Quantity (wt-%)	O (wt-%)	P (wt-%)	Ca (wt-%)
Oxyapatite	QOxyapatite	6.05	40.54	18.84	40.62
alphaTCP	QalphaTCP	62.99	41.27	19.97	38.76
betaTCP	QbetaTCP	30.95	41.27	19.97	38.76
Weighted total		99.99	41.22	19.90	38.87

Calculates the refined chemical composition based on:

- Refined atomic sites (scattering factors, site occupancy factors)
- Refined phase quantities

Not recommended as a chemical analysis,
but useful to validate refinement results by
comparison with chemical analysis (ICP, XRF)

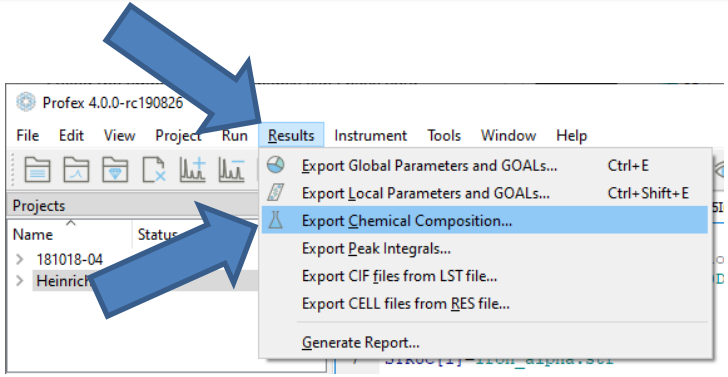
Example 2: Refined Chemical Composition



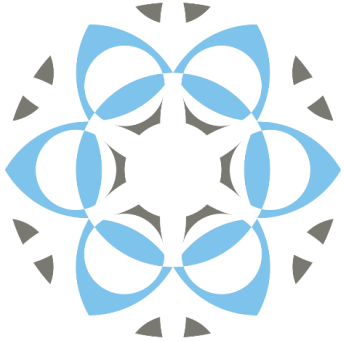
Refined Chemical Composition

Chemical Composition

	Quantity Goal	Phase Quantity (wt-%)	SiO2 (wt-%)	SO3 (wt-%)	Fe2O3 (wt-%)	ZnO (wt-%)	In2O3 (wt-%)
CRISTOBALITE	Qcristobalite	8.17	100.00	0.00	0.00	0.00	0.00
Indite	QIndite	14.20	0.00	47.25	11.78	0.00	40.97
Iron_alpha	Qironalpha	0.84	0.00	0.00	100.00	0.00	0.00
Magnetite	QMagnetite	0.10	0.00	0.00	100.00	0.00	0.00
Sphalerite	QSphalerite	67.60	0.00	49.59	0.00	50.41	0.00
Wurtzite2H	QWurtzite2H	9.14	0.00	49.59	0.00	50.41	0.00
Weighted total		100.05	8.17	44.76	2.62	38.68	5.82



Up Next and Tomorrow: New Features in Profex 4



- GUI changes
- Search / Match
- Peak detection
- Interaction with QualX / Match!

- Electron-density maps
- Drawing crystal structures with Vesta / Mercury
- Customizing report layouts

RMS