

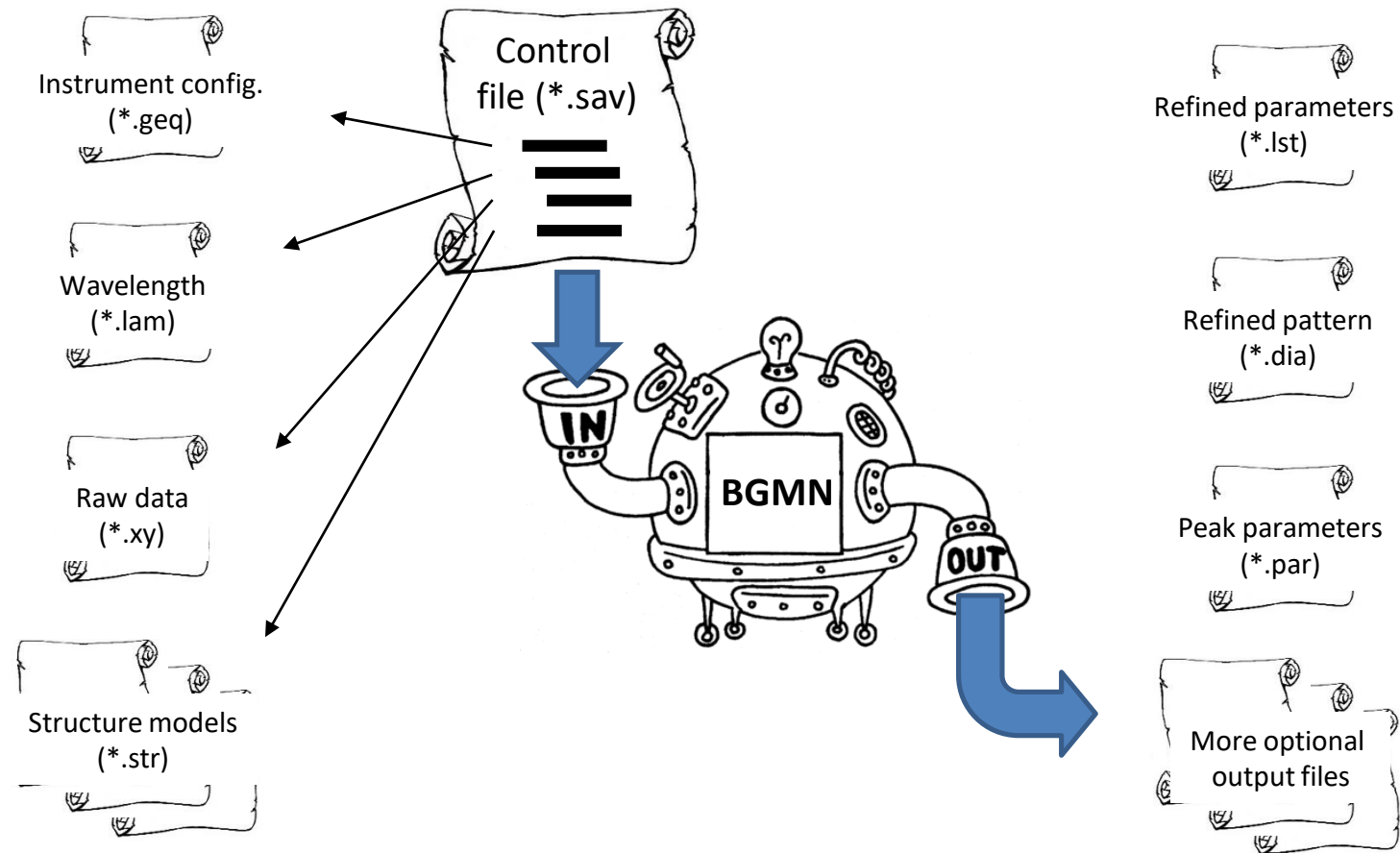
BGMN/Profex User Meeting 2019

Profex – A Graphical User Interface for BGMN

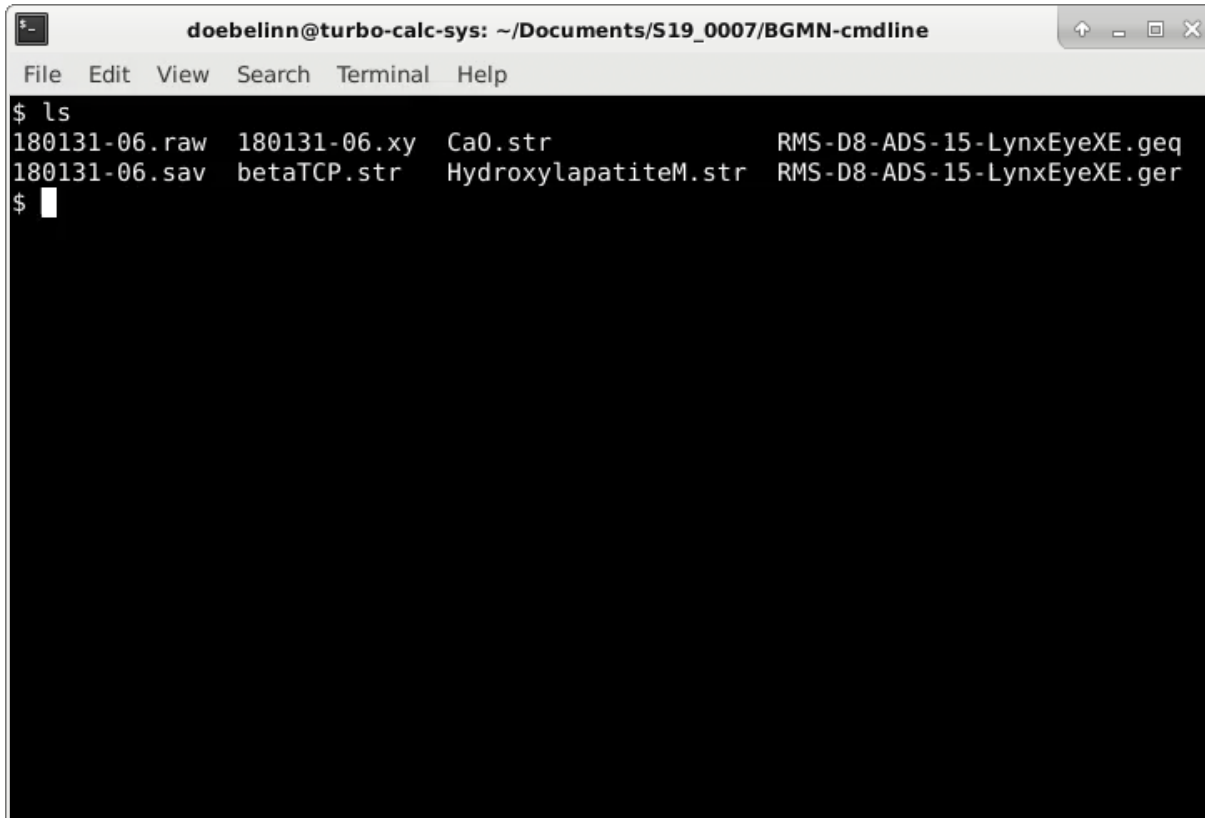
Nicola Döbelin

RMS Foundation, Bettlach, Switzerland

BGMN: Based on Text Files



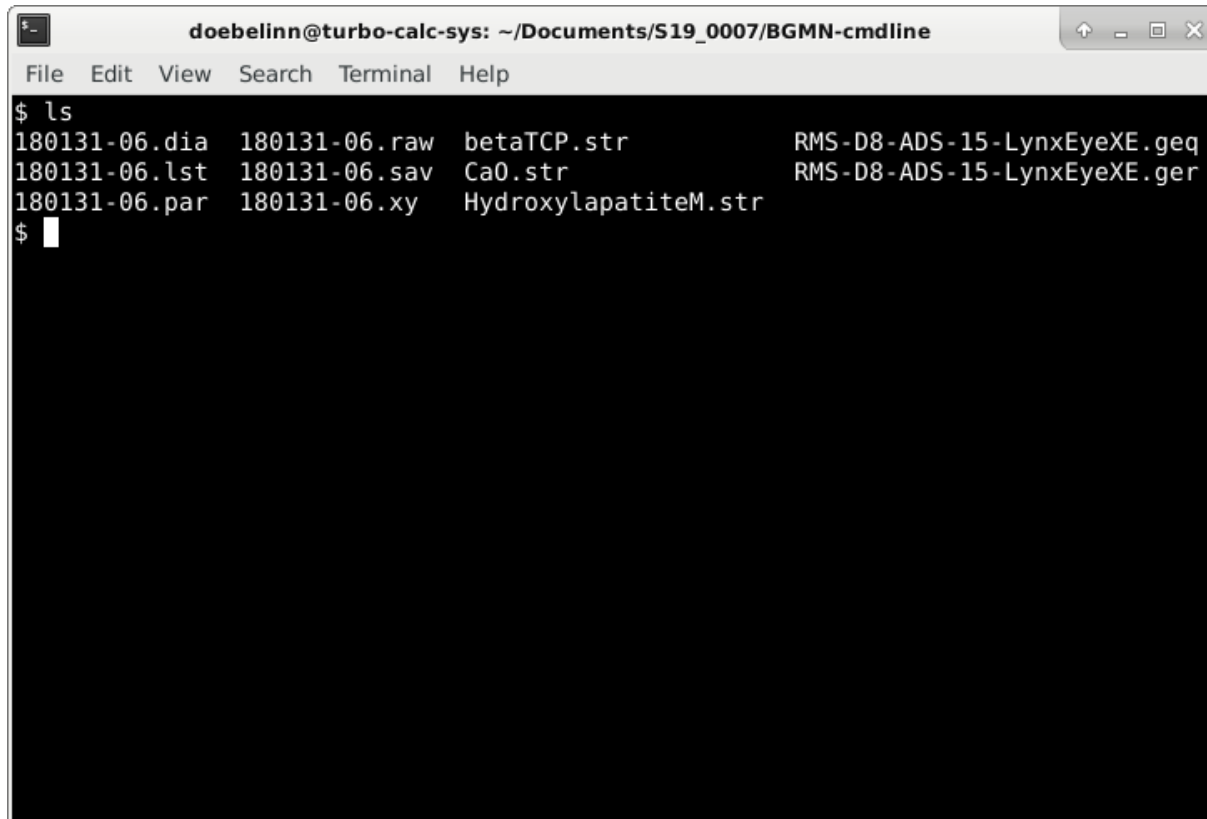
BGMN Command Line Application



A terminal window titled "doebelinn@turbo-calc-sys: ~/Documents/S19_0007/BGMN-cmdline" with a menu bar containing "File", "Edit", "View", "Search", "Terminal", and "Help". The terminal shows the command "\$ ls" and its output:

```
$ ls
180131-06.raw  180131-06.xy  Ca0.str          RMS-D8-ADS-15-LynxEyeXE.geq
180131-06.sav  betaTCP.str   HydroxylapatiteM.str RMS-D8-ADS-15-LynxEyeXE.ger
$
```

BGMN Command Line Application



A terminal window titled "doebelinn@turbo-calc-sys: ~/Documents/S19_0007/BGMN-cmdline" with a menu bar containing "File", "Edit", "View", "Search", "Terminal", and "Help". The terminal shows the command "\$ ls" and its output:

```
$ ls
180131-06.dia  180131-06.raw  betaTCP.str      RMS-D8-ADS-15-LynxEyeXE.geq
180131-06.lst  180131-06.sav  Ca0.str          RMS-D8-ADS-15-LynxEyeXE.ger
180131-06.par  180131-06.xy   HydroxylapatiteM.str
```

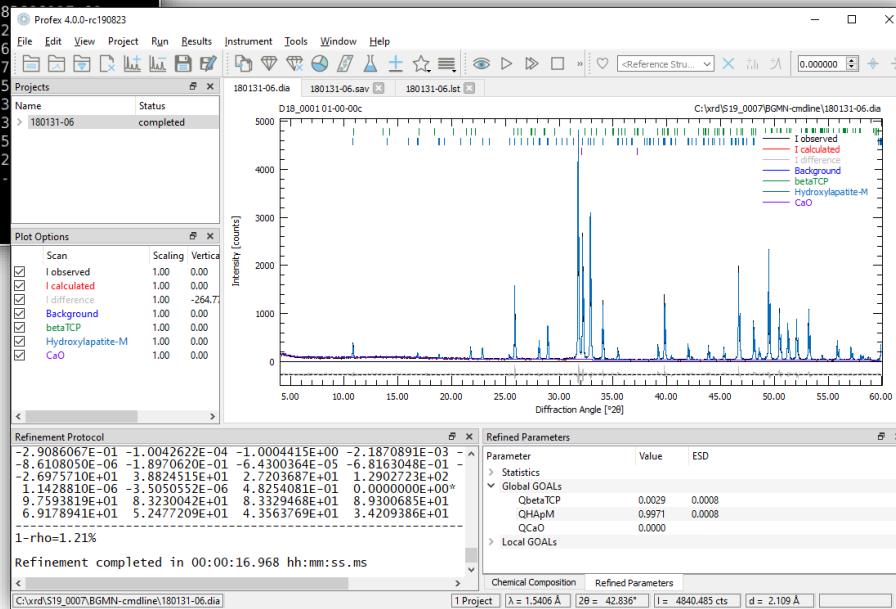
The prompt "\$" is followed by a cursor.

Graphical User Interfaces for BGMN

```
doebelinn@turbo-calc-sys: ~/Documents/S19_0007/BGMN-cmdline
File Edit View Search Terminal Help
6.9204168E+01 5.2599022E+01 4.3629372E+01 3.4411554E+01 3.2346232E+01
-----
Rietveld refinement with 4573 data points and 55 parameters
*****
-----
N= 55 IT= 550
  0 4.761710E+03
 1.0449457E+00 3.7400423E+00 1.8528587E-04 9.4198080E-01 1.8850508E+00
 6.8809112E-01 1.2001831E+02 8.1741676E-09 -1.1403040E+01 -2.1563404E+00
-1.3767821E-03 -7.7343888E-01 8.3457133E-04 -4.5722867E+00 -3.8
 5.4592082E-04 -1.7086651E+00 2.9780903E-03 -2.5730510E-01 1.2
-7.1725634E-01 6.9836784E-04 -4.8340643E+00 -1.8733465E-01 7.6
-2.9036163E-01 -1.4626429E-04 -9.1136496E-01 6.6186806E-03 -1.7
 7.3623688E-05 -1.8603958E-01 -1.7831216E-04 -6.6687938E-01 9.5
-2.7091850E+01 4.9188340E+01 3.4555285E+01 1.3025047E+02 2.3
 5.2751596E-07 -1.2619549E-06 4.8187610E-01 0.0000000E+00* 1.3
 9.7642048E+01 8.3169611E+01 8.3361624E+01 8.9335683E+01 8.5
 6.9204168E+01 5.2599022E+01 4.3629372E+01 3.4411554E+01 3.2
-----
1-rho=1.22%
unable to write config-file bgmn.cfg
$
```

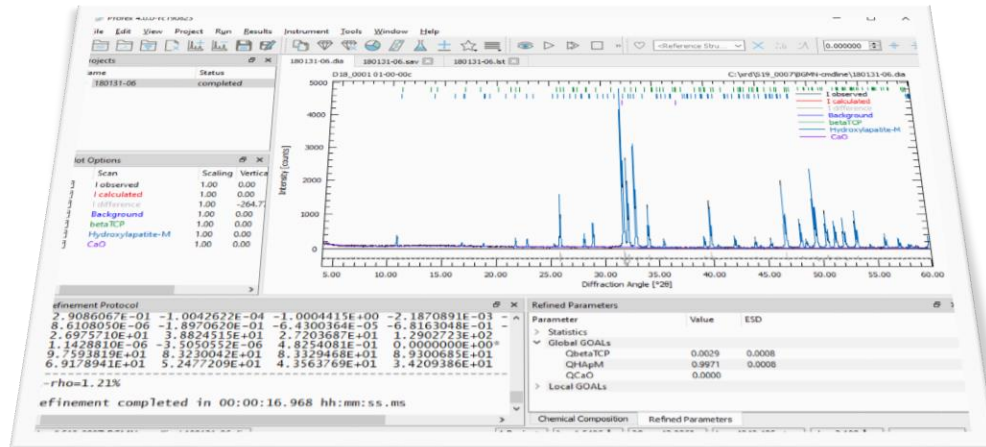
← BGMN can be used from a command shell. No user interface is required.

But much more convenient with a user interface →



Profex – A Graphical User Interface for BGMN

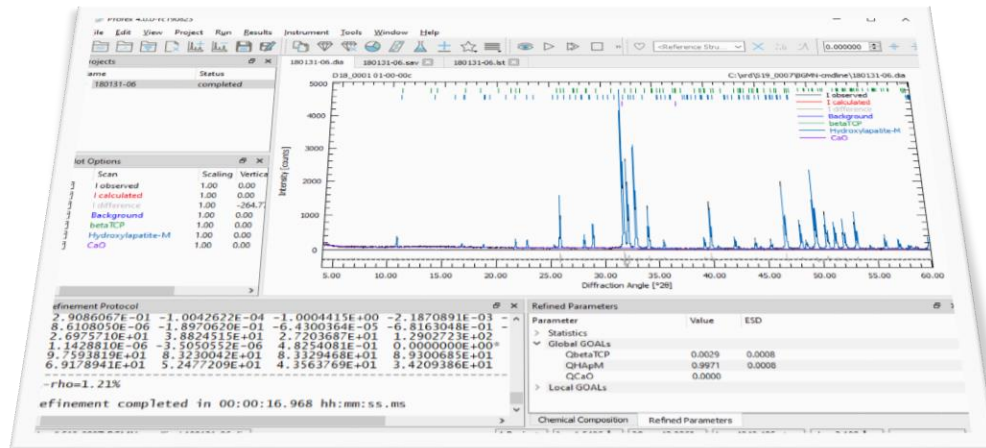
Developer: Nicola Döbelin (private)
License: GPL v2 or later (open source)
Founded in: 2003
Platforms: Windows 7 / 8 / 8.1 / 10
Mac OS X 10.9 -10.14 (64bit)
Linux
Rietveld Backends: BGMN, Fullprof.2k
Website: <http://www.profex-xrd.org>
Current stable version: 4.0.0



Profex – A Graphical User Interface for BGMN

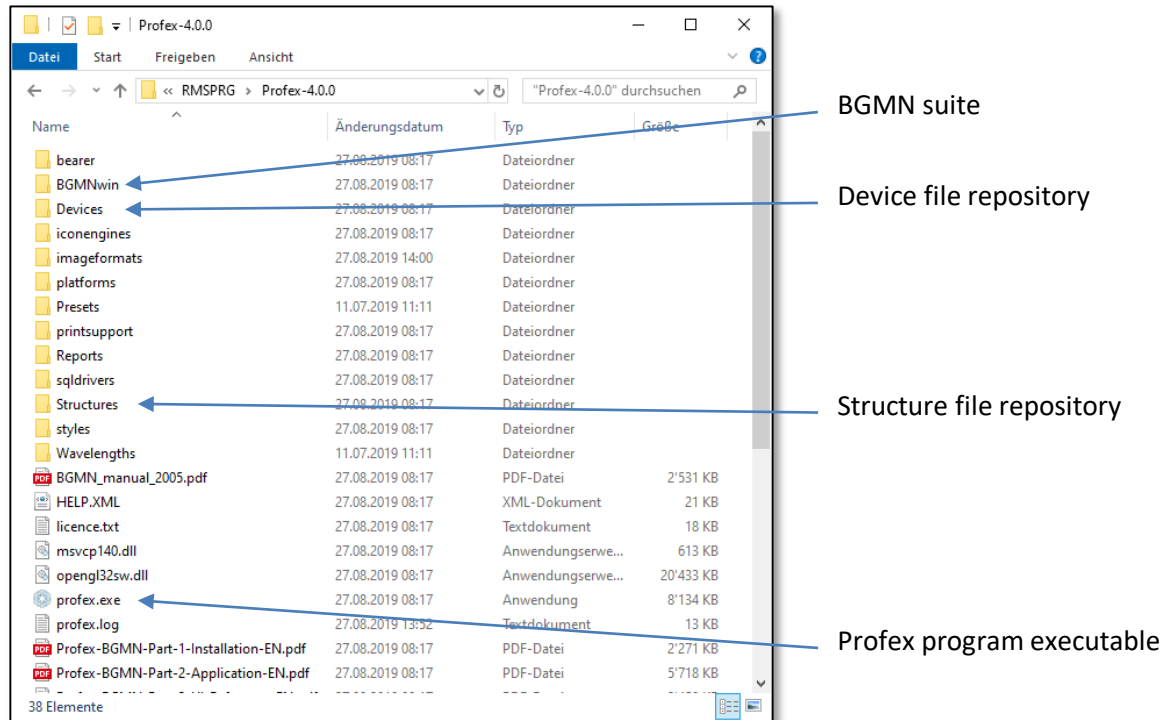
Version 4.0.0:

- 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
 - ...



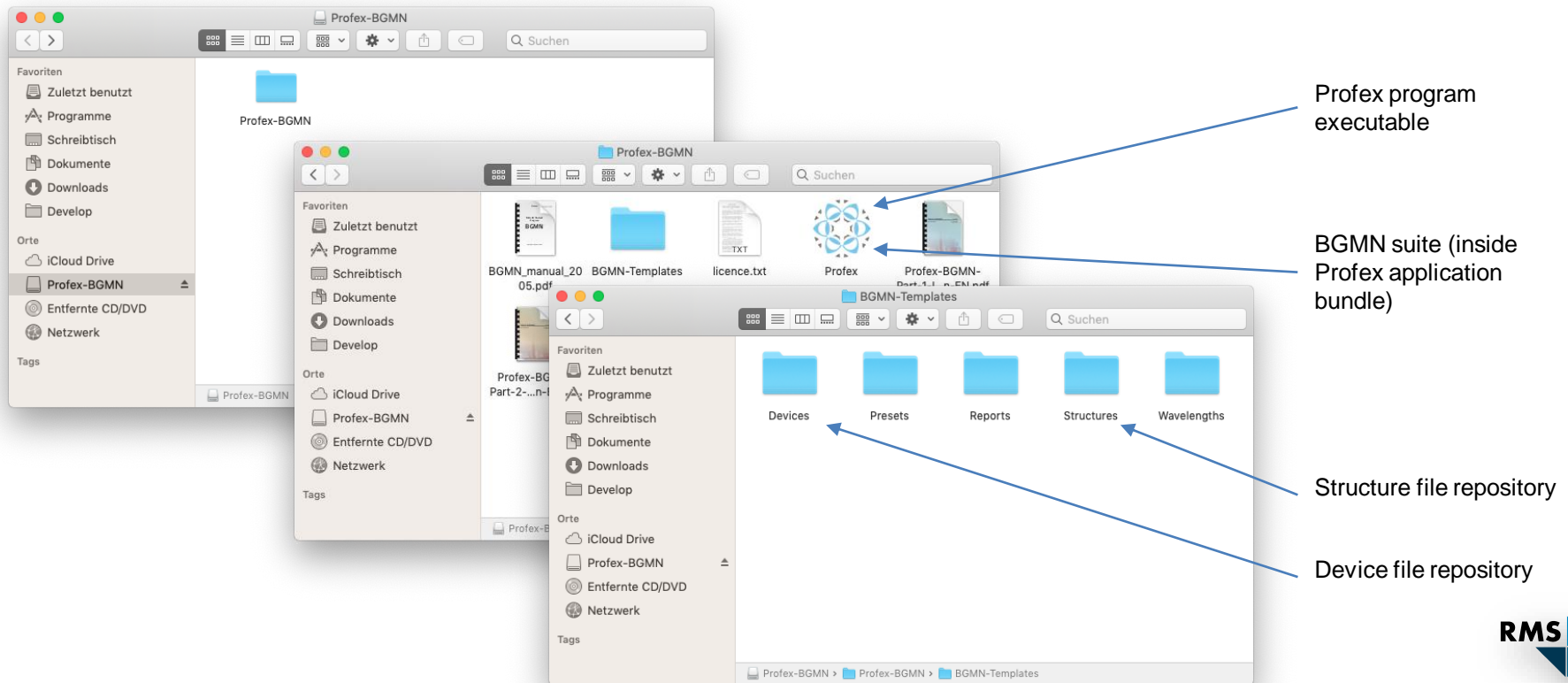
Installing Profex

- 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



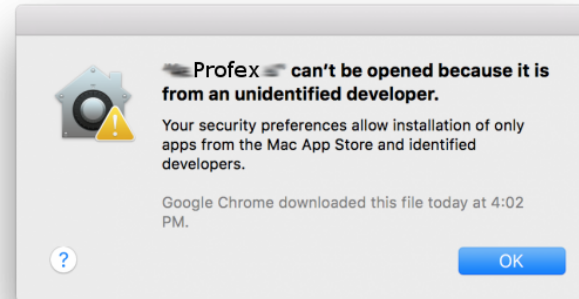
Profex: First Start Security Warnings

Windows

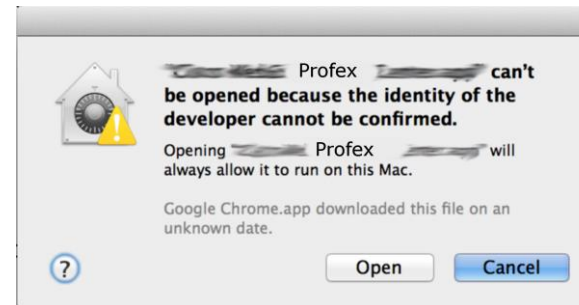


«More Info» → «Run anyway»

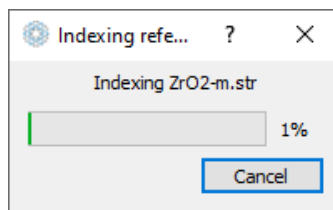
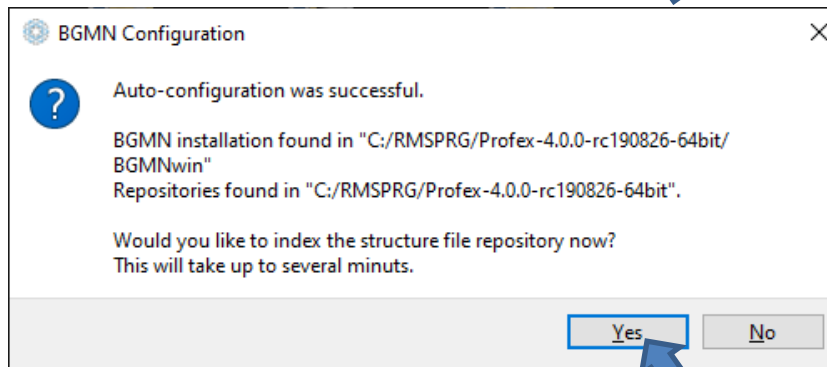
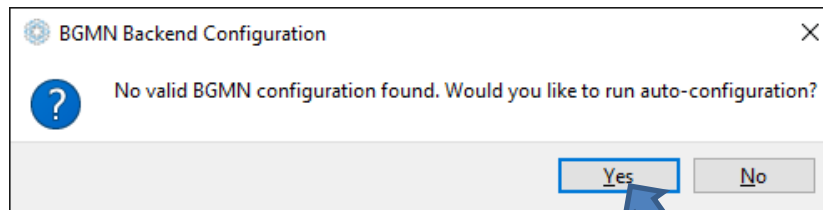
OS X:



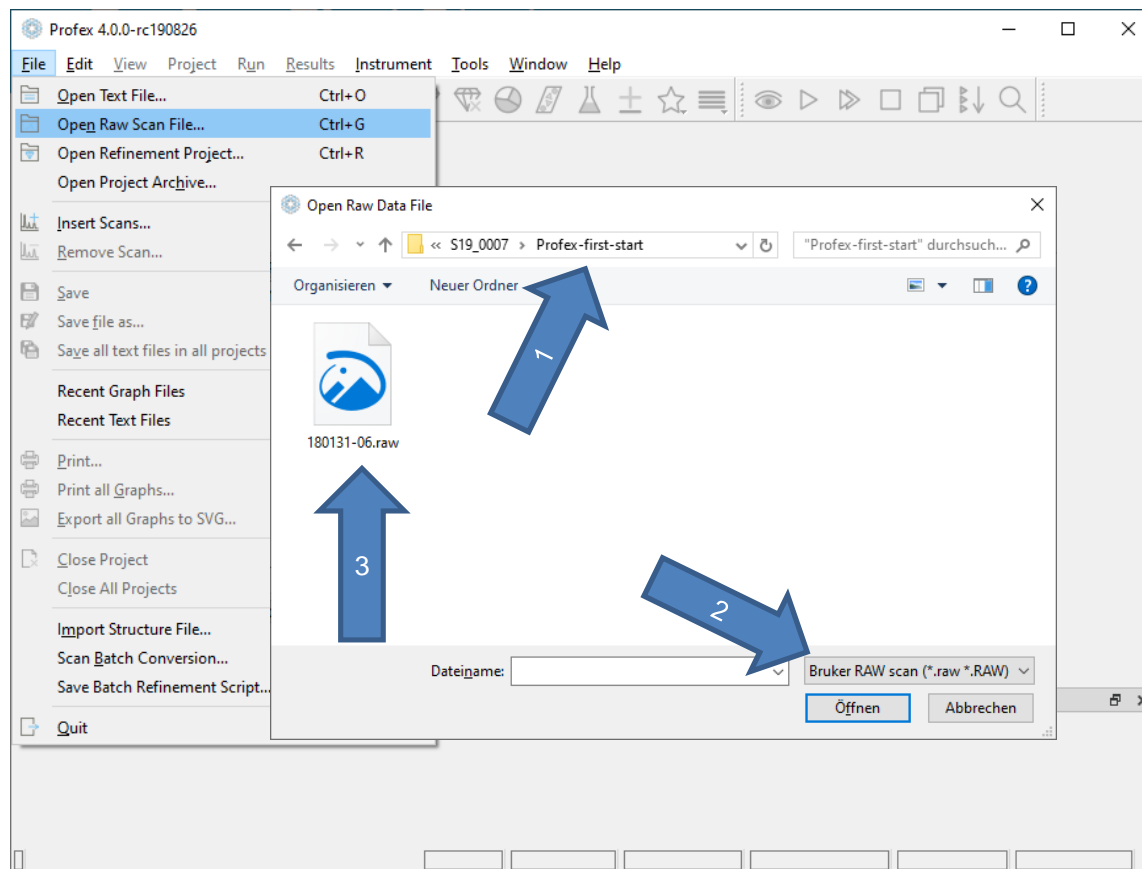
Ctrl + Click on Profex → "Open"



«Open»



Profex: First Start



Profex: First Start



Plot area
(cannot be closed)

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

Profex: First Start

Profex 4.0.0-rc190826

File Edit View Project Run Results Instrument Tools **Window** Help

Projects

Name	Status
> 180131-06	idle

180131-06.raw

D18_000

intensity [counts]

5000

4000

3000

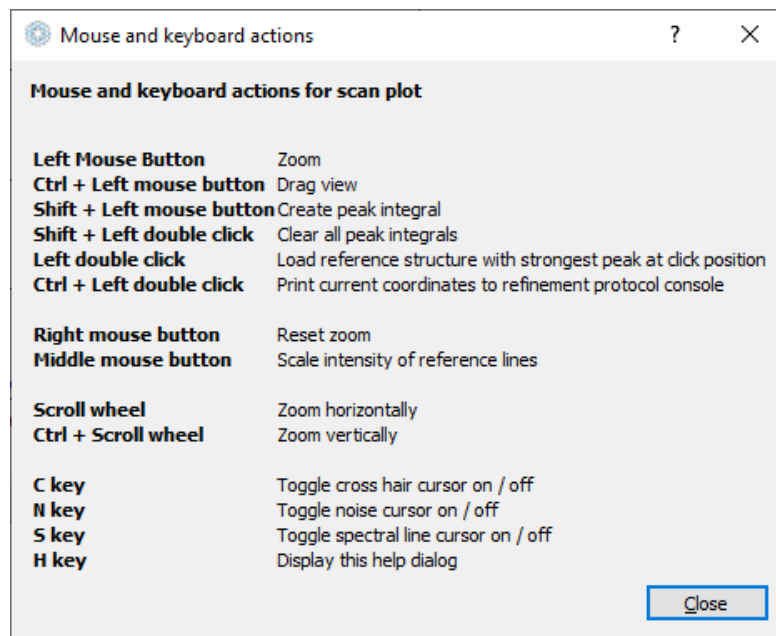
2000

D18_0001 01-00-00c

- Projects
- Plot Options
- Refinement Protocol
- Chemical Composition
- Context Help
- Convergence Progress
- Peak Integrals
- Peak List
- Search/Match Phases
- Refined Parameters

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

Help → Mouse and Keyboard Commands:



Indexed Reference Structures

Select Reset

The screenshot displays the Profex 4.0.0-rc190826 software interface. The main window shows a diffraction pattern plot with Intensity [counts] on the y-axis (0 to 5000) and Diffraction Angle [2θ] on the x-axis (5.00 to 60.00). The plot title is 'D18_0001 01-00-00c'. A blue line represents the experimental data, and green lines represent the reference hkl lines. A dropdown menu is open, listing various mineral phases: Anorthite, ANALCIMC, Anataase, Andalusite, Anglesite, Anhydrite, Ankerit02, Ankerit05, Ankerit07, ANNITE, and Anorthite. The 'Anorthite' entry is highlighted in blue. A red 'X' icon in the dropdown is circled in red, labeled 'Reset'. A green arrow points to the 'Anorthite' entry, labeled 'Select'. Another green arrow points to the reference hkl lines on the plot, labeled 'Reference hkl lines'.

Projects

Name	Status
> 180131-06	idle

Plot Options

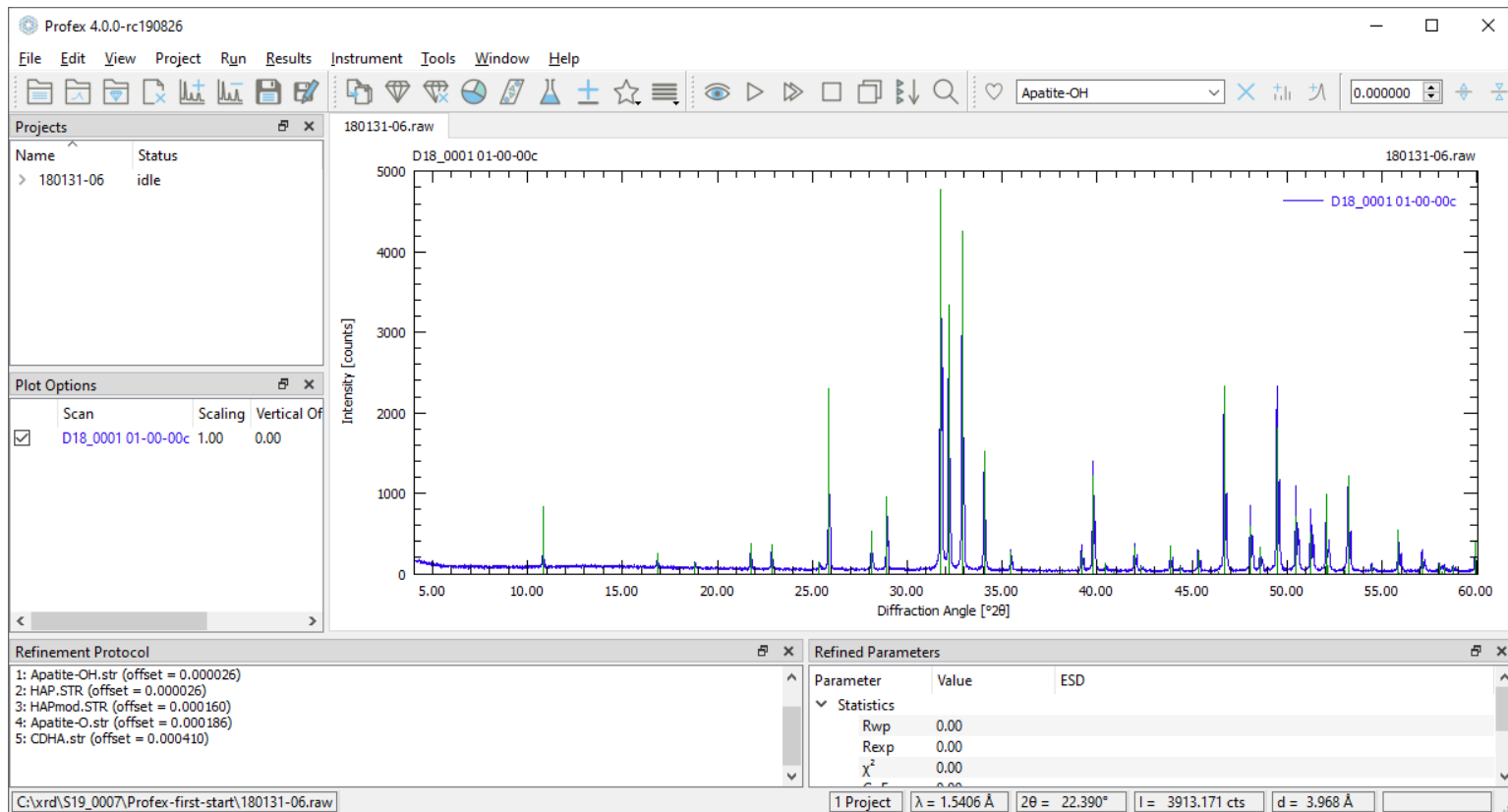
Scan	Scaling	Vertical Of
<input checked="" type="checkbox"/> D18_0001 01-00-00c	1.00	0.00

Refined Parameters

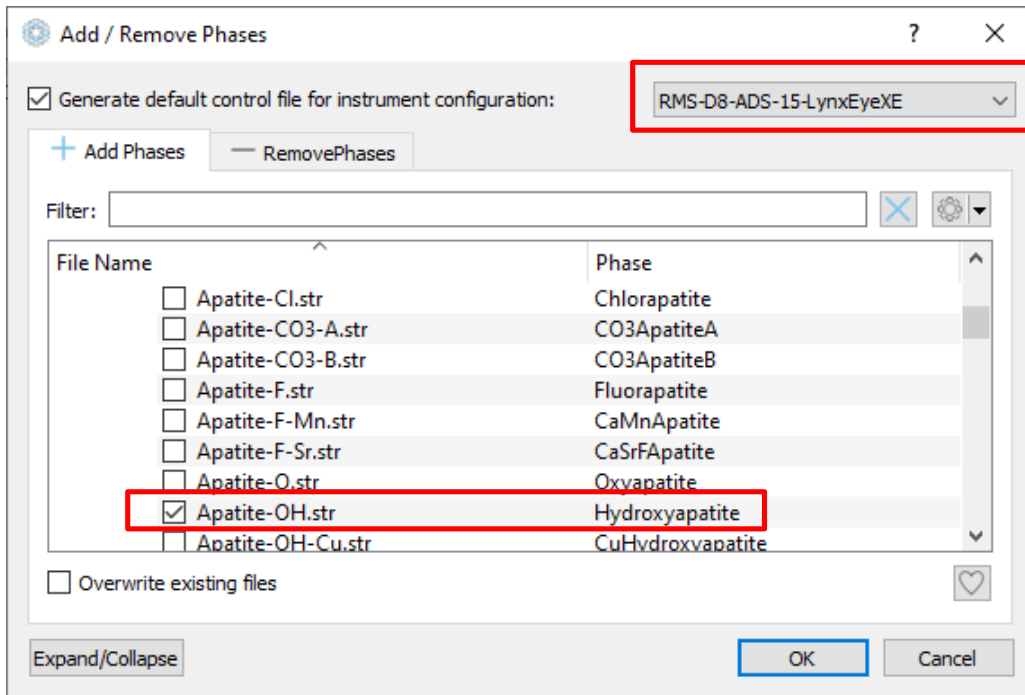
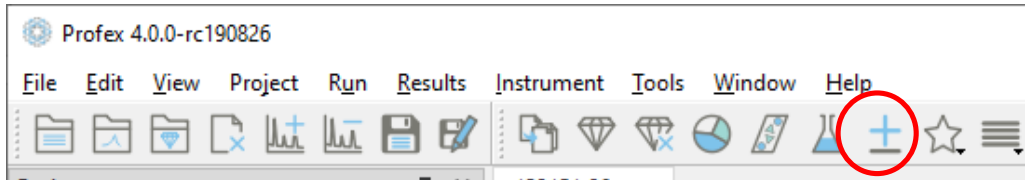
Parameter	Value	ESD
Statistics		
Rwp	0.00	
Rexp	0.00	
χ^2	0.00	
GOF	0.00	

1 Project $\lambda = 1.5406 \text{ \AA}$ $2\theta = 0.000^\circ$ $I = 0.000 \text{ cts}$ $d = 0.000 \text{ \AA}$

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

The screenshot displays the Profex 4.0.0-rc190826 software interface. The main window shows the 'Tools' menu highlighted with a blue arrow. The 'Refinement Protocol' section is visible, listing several refinement steps with their respective offsets.

Refinement Protocol:

- 1: Apatite-OH.str (offset = 0.000026)
- 2: HAP_STR (offset = 0.000026)
- 3: HAPmod.STR (offset = 0.000160)
- 4: Apatite-O.str (offset = 0.000186)
- 5: CDHA.str (offset = 0.000410)

The main window also displays the following parameters:

```
1 % SampleID: D18_0001 01-00-00c
2 % Theoretical instrumental function
3 VERZERR=RMS-D8-ADS-15-LynxEyeXE.geq
4 % Wavelength
5 LAMBDA=CU
6 % Phases
7 STRUC[1]=Apatite-OH.str
8 % Measured background
9 UNT=RMS-D8-ADS-15-LynxEyeXE-bkgr.xy
10 RU=10
11 % Measured data
12 VAL[1]=180131-06.xy
13 % Minimum Angle (2theta)
14 WMIN=10
15 % Maximum Angle (2theta)
16 % WMAX=60
17 % Result list output
18 LIST=180131-06.lst
19 % Peak list output
20 OUTPUT=180131-06.par
21 % Diagram output
22 DIAGRAMM=180131-06.da
23 % Global parameters for zero point and sample displacement
24 EPS1=0
25 PARAM[1]=EPS2=0_-0.01^0.01
26 EPS3=0
27 alpha3ratio=0.020
28 betaratio=0.005
29 NTHREADS=8
30 PROTOKOLL=Y
```

An inset window shows a file explorer view of the project directory 'Profex-first-start' containing the following files:

- 180131-06.raw
- Apatite-OH.str
- RMS-D8-ADS-15-LynxEyeXE.geq
- RMS-D8-ADS-15-LynxEyeXE.ger
- RMS-D8-ADS-15-LynxEyeXE.sav
- RMS-D8-ADS-15-LynxEyeXE-bkgr.xy

Step 3: Release parameters for refinement

Open all structure files

The screenshot shows the Profex 4.0.0-rc190826 software interface. The 'Instrument' menu is highlighted with a red circle. The main window displays a list of parameters for Hydroxyapatite refinement, including unit cell parameters (A, B, C), crystallite size (B1), and scale factor (GEWICHT=SPHAR4).

```

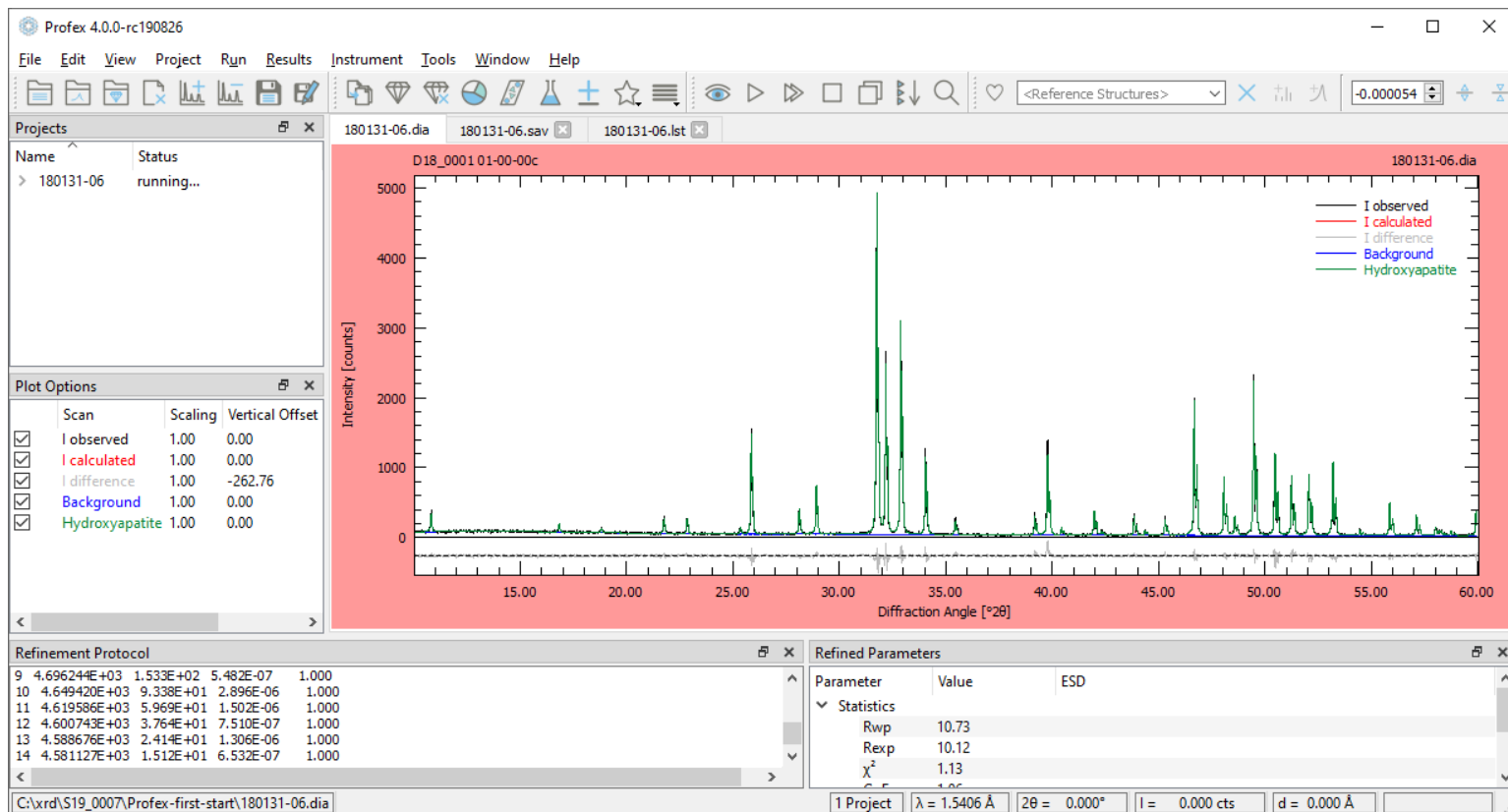
1 PHASE=Hydroxyapatite // 01-074-0565]
2 MineralName=Hydroxylapatite //
3 Formula=Ca5_(PO4)3_(OH) //
4 SpacegroupNo=176 HermannMauguin=P6_3/m //
5 PARAM=A=0.9424_0.9330^0.9518 PARAM=C=0.6879_0.6810^0.6948 //
6 RP=4 k1=0 k2=0 B1=ANISO^0.05 GEWICHT=SPHAR4 //
7 GOAL=GrainSize(0,0,1) //
8 GOAL=GrainSize(1,0,0) //
9 GOAL:Hydroxyapatite=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1)
10 E=CA Wyckoff=f x=0.3333 y=0.6667 z=0.0015 TDS=0.00664290
11 E=CA Wyckoff=h x=0.2468 y=0.9934 z=0.2500 TDS=0.00567436
12 E=P Wyckoff=h x=0.3987 y=0.3685 z=0.2500 TDS=0.00477426
13 E=O Wyckoff=h x=0.3284 y=0.4848 z=0.2500 TDS=0.00953535
14 E=O Wyckoff=h x=0.5873 y=0.4651 z=0.2500 TDS=0.01014069
15 E=O Wyckoff=i x=0.3437 y=0.2579 z=0.0702 TDS=0.01499127
16 E=O(0.5000) Wyckoff=e x=0.0000 y=0.0000 z=0.1950 TDS=0.00000000
17 E=H(0.5000) Wyckoff=e x=0.0000 y=0.0000 z=0.0608 TDS=0.02947459
18

```

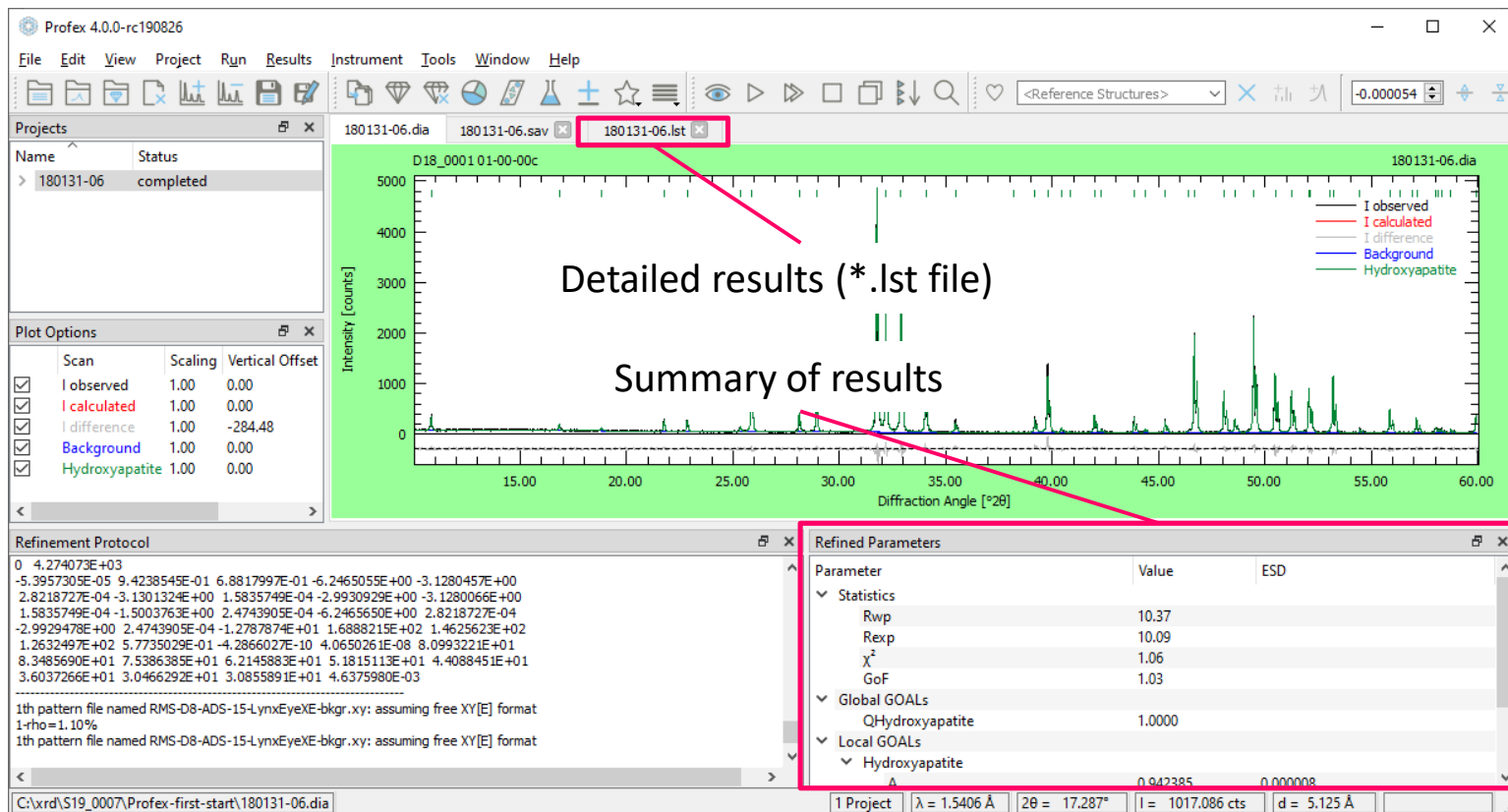
Already released for refinement:

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

Step 4: Run the refinement



Results



Open «Window → Context Help»

The screenshot shows the Profex 4.0.0-rc190826 software interface. The main window displays a list of parameters for Hydroxyapatite, including k_2 . The Context Help window is open, providing detailed information about the k_2 parameter.

Context Help

using the default setting

$$B2 = k1 * \text{sqr}(B1) + k2 * \text{sqr}(sk)$$

k_2 defines the square of the micro strain. Special settings for anisotropic strain are

$k_2 = \text{ANISO}$

which means

$k_2 = \text{ANISOSQR}$

and for complicated cases

$k_2 = \text{ANISO4}$

1. Place the cursor on a parameter (here: k_2)
2. Press «F1» key

Release Micro-Strain for refinement

The screenshot shows the Profex 4.0.0-rc190826 software interface. The main window displays the Apatite-OH.str file with the following content:

```

1 PHASE=Hydroxyapatite // 01-074-0565
2 MineralName=Hydroxylapatite //
3 Formula=Ca5_(PO4)3_(OH) //
4 SpacegroupNo=176 HermannMauguin=P6_3/m //
5 PARAM=A=0.9424_0.9330^0.9518 PARAM=C=0.6879_0.6810^0.6948 //
6 RP=4 k1=0 k2=0.31=ANISO^0.05_GEWICHT=SPHAR4 //
7 GOAL=GrainS
8 GOAL=GrainS
9 GOAL:Hydrox
10 E=CA Wyckoff 0015 TDS=0.00664290
11 E=CA Wyckoff 2500 TDS=0.00567436
12 E=P Wyckoff 500 TDS=0.00477426
13 E=O Wyckoff 500 TDS=0.00953535
14 E=O Wyckoff 500 TDS=0.01014069
15 E=O Wyckoff 702 TDS=0.01499127
16 E=O(0.5000) 00 z=0.1950 TDS=0.00000000
17 E=H(0.5000) 00 z=0.0608 TDS=0.02947459
18

```


A context menu is open over the parameter «k2» in line 6. The menu items are:

- Undo
- Redo Ctrl+Y
- Cut
- Copy
- Paste
- Delete
- Select All Ctrl+A
- Refine isotropically
- Refine anisotropically
- Fix parameter
- Comment line

The 'Refine isotropically' and 'Refine anisotropically' options are highlighted with a red box.

The left sidebar shows the 'Projects' panel with '180131-06' completed and the 'Plot Options' panel with the following settings:

Scan	Scaling	Vertical Offset
<input checked="" type="checkbox"/> I observed	1.00	0.00
<input checked="" type="checkbox"/> I calculated	1.00	0.00
<input checked="" type="checkbox"/> I difference	1.00	-284.48
<input checked="" type="checkbox"/> Background	1.00	0.00
<input checked="" type="checkbox"/> Hydroxyapatite	1.00	0.00

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

The screenshot shows the Profex 4.0.0-rc190826 software interface. The main window displays the refinement parameters for Hydroxyapatite. A context menu is open over the refinement parameters, with the option "Refine isotropically" highlighted. The parameters are as follows:

```

1 PHASE=Hydroxyapatite // 01-074-0565
2 MineralName=Hydroxylapatite //
3 Formula=Ca5_(PO4)3_(OH) //
4 SpacegroupNo=176 HermannMauguin=P6_3/m //
5 PARAM=A=0.9424 0.9330^0.9518 PARAM=C=0.6879_0.6810^0.6948 //
6 RP=4 k1=0 k2=0_B1=ANISO^0.05_GEWICHT=SPHAR4 //
7 GOAL=GrainS
8 GOAL=GrainS
9 GOAL:Hydrox
10 E=CA Wyckof 0015 TDS=0.00664290
11 E=CA Wyckof 2500 TDS=0.00567436
12 E=P Wyckoff 500 TDS=0.00477426
13 E=O Wyckoff 500 TDS=0.00953535
14 E=O Wyckoff 500 TDS=0.01014069
15 E=O Wyckoff 702 TDS=0.01499127
16 E=O (0.5000) 00 z=0.1950 TDS=0.00000000
17 E=H (0.5000) 00 z=0.0608 TDS=0.02947459
18

```

The context menu options are:

- Undo
- Redo Ctrl+Y
- Cut
- Copy
- Paste
- Delete
- Select All Ctrl+A
- Refine isotropically**
- Refine anisotropically
- Fix parameter
- Comment line

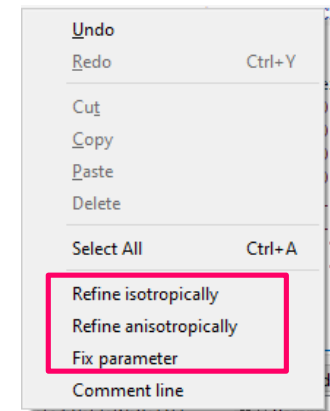
The "Refine isotropically" option is highlighted with a red box. The software interface also shows a "Plot Options" panel on the left with the following settings:

Scan	Scaling	Vertical Offset
<input checked="" type="checkbox"/> Observed	1.00	0.00
<input checked="" type="checkbox"/> Calculated	1.00	0.00
<input checked="" type="checkbox"/> Difference	1.00	-284.48
<input checked="" type="checkbox"/> Background	1.00	0.00
<input checked="" type="checkbox"/> Hydroxyapatite	1.00	0.00

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

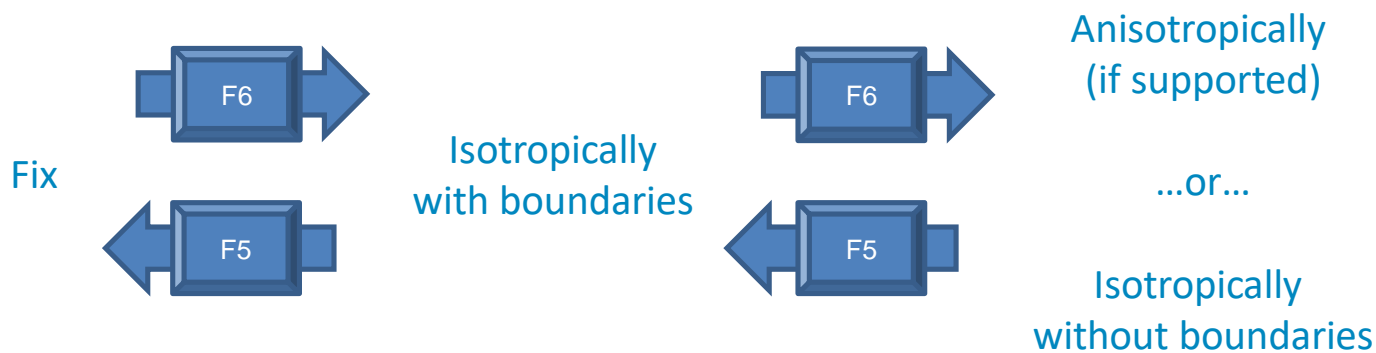
Releasing / Fixing Parameters for Refinement

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

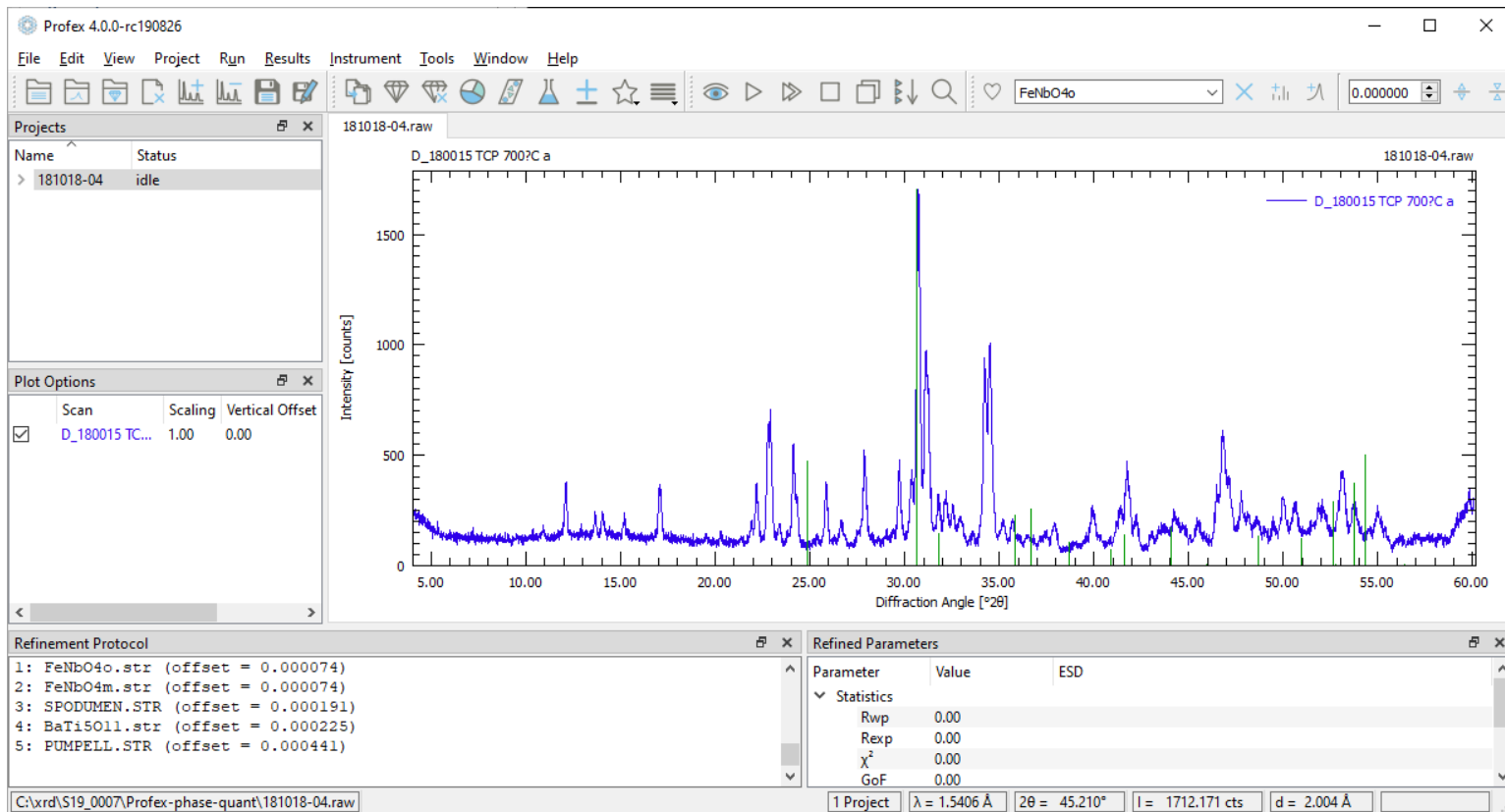


Alternatively:

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 \neq strongest peak (highest integrated intensity)

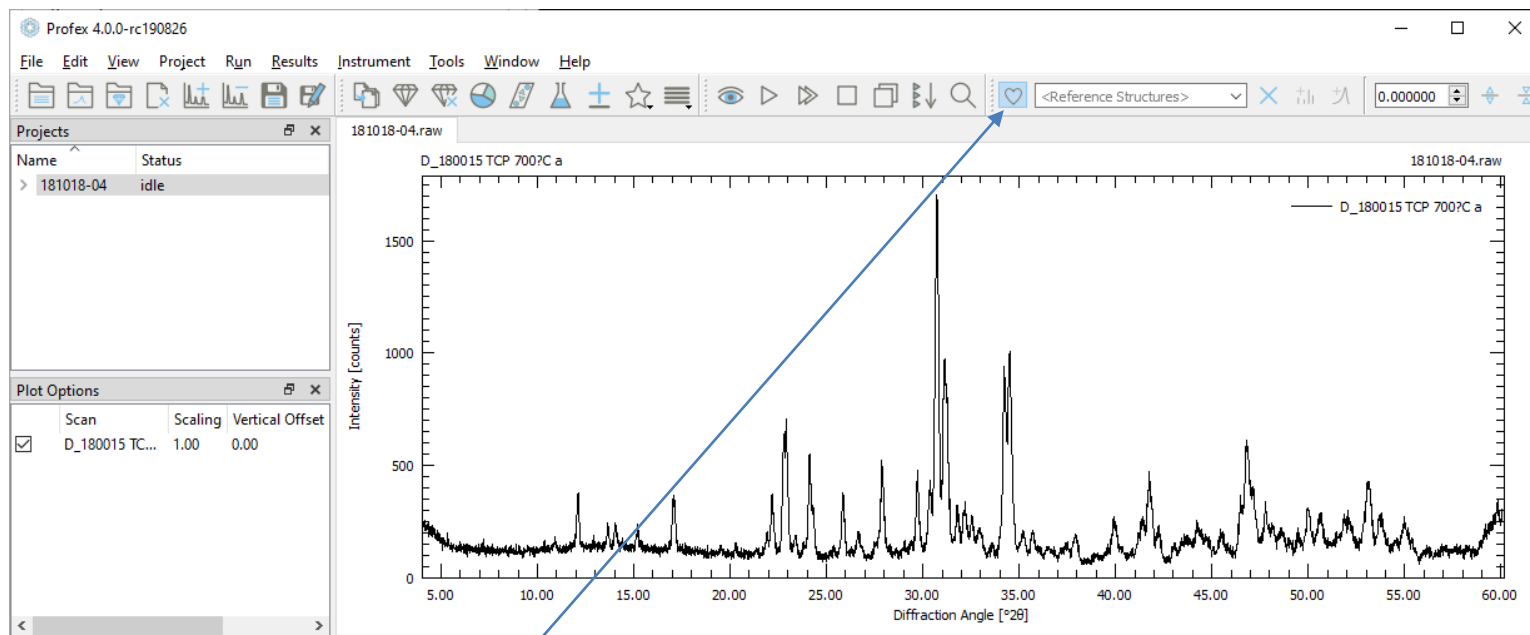
Example 2: Favorites / Phase quantification

The screenshot shows the Profex 4.0.0.26 software interface. The 'File' menu is open, and the 'Preferences...' option is highlighted. The 'Preferences' dialog box is open, showing the 'BGMN' section. The 'Favorites' group is expanded, and the 'Phosphate' group is highlighted with a red box. The 'Phosphate' group contains the following items:

File Name	Phase
<input type="checkbox"/> C:\RMSPRG\Profex-4.0.0...	
<input type="checkbox"/> Alumina-Titania-Zirc...	
<input type="checkbox"/> amorphPeak.str	/Users/doebelinn/AppData/Local/Temp/a...
<input type="checkbox"/> BGMN	
<input type="checkbox"/> Cement	
<input type="checkbox"/> Ceramics	
<input type="checkbox"/> MetalsAlloysOxides	
<input type="checkbox"/> Minerals	
<input type="checkbox"/> Organic	
<input type="checkbox"/> Phosphate	
<input type="checkbox"/> SiC	

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

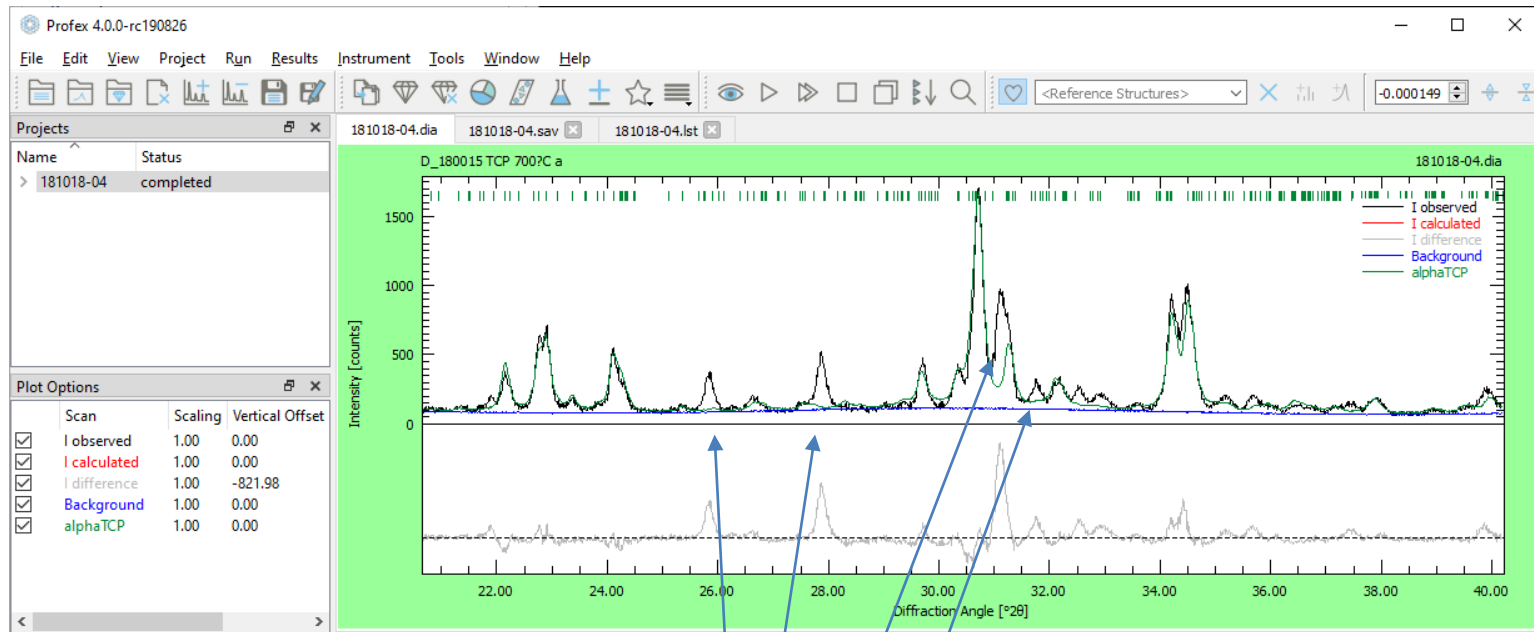
The screenshot displays the Profex 4.0.0-rc190826 software interface. The main window shows a powder XRD pattern for the file 'D_180015 TCP 700°C a'. The y-axis is 'Intensity [counts]' ranging from 0 to 1500, and the x-axis is 'Diffrac' ranging from 5.00 to 30.0. A red circle highlights the '+' icon in the toolbar, with an arrow pointing to the 'Add Phases' button in the 'Add / Remove Phases' dialog box. The dialog box is open, showing a list of reference phases. The 'TCP-alpha.str' phase is selected, and its corresponding phase name 'alphaTCP' is listed. The dialog also includes options for generating a default control file, overwriting existing files, and showing favorite phases only.

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

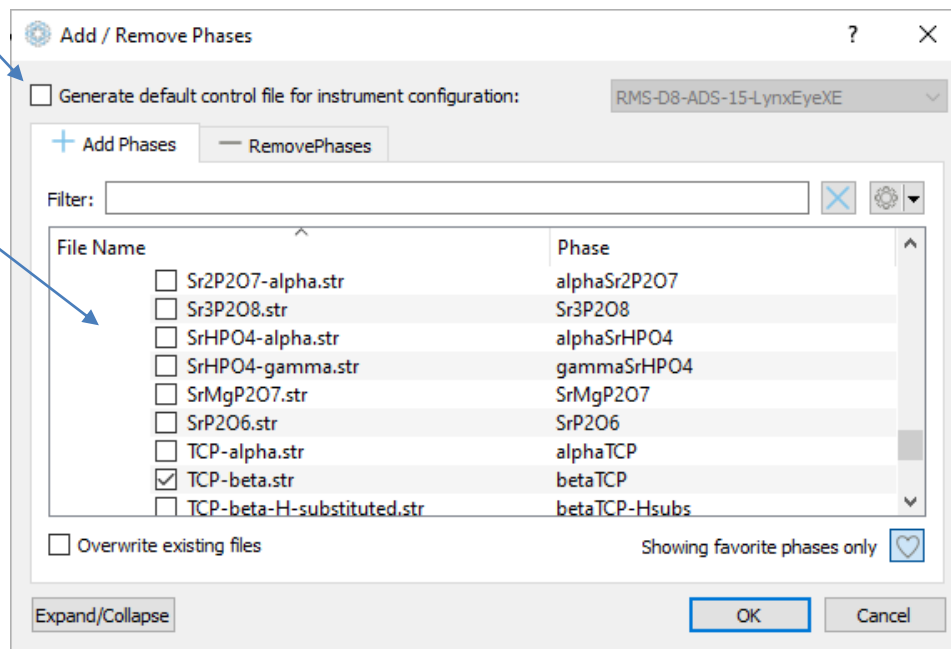


More unidentified phases

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

The screenshot displays the Profex 4.0.0-rc190826 software interface. The main window shows the project settings for '181018-04.dia'. The 'Phases' section is highlighted with a red box, showing the following settings:

```
7 STRUC[1]=TCP-alpha.str
8 STRUC[2]=Apatite-O.str
9 STRUC[3]=TCP-beta.str
```

The 'Plot Options' section is also visible, showing the following settings:

Scan	Scaling	Vertical Offset
<input checked="" type="checkbox"/> I observed	1.00	0.00
<input checked="" type="checkbox"/> I calculated	1.00	0.00
<input checked="" type="checkbox"/> I difference	1.00	-821.98
<input checked="" type="checkbox"/> Background	1.00	0.00
<input checked="" type="checkbox"/> alphaTCP	1.00	0.00

The 'Refinement Protocol' section is empty. The 'Refined Parameters' section shows the following statistics:

- Statistics
- Rwp
- Rexp
- χ^2
- GoF

The file explorer window shows the project directory 'Profex-phase-quant' with the following files:

- 181018-04.dia
- 181018-04.lst
- 181018-04.par
- 181018-04.raw
- 181018-04.sav
- 181018-04.xy
- Apatite-O.str (highlighted with a red arrow)
- RMS-D8-ADS-15-LynxEyeXE.geq
- RMS-D8-ADS-15-LynxEyeXE.ger
- RMS-D8-ADS-15-LynxEyeXE.sav
- RMS-D8-ADS-15-LynxEyeXE.tpl
- RMS-D8-ADS-15-LynxEyeXE-bkgr.xy
- TCP-alpha.str
- TCP-beta.str (highlighted with a red arrow)

The status bar at the bottom of the Profex window shows the file path: 'C:\xrd\S19_0007\Profex-phase-quant\181018-04.sav' and '1 Project'.

Example 2: Favorites / Phase quantification

The screenshot shows the Profex 4.0.0-rc190826 software interface. The main window displays a list of parameters for phase quantification. A red box highlights the following lines (34-42):

```

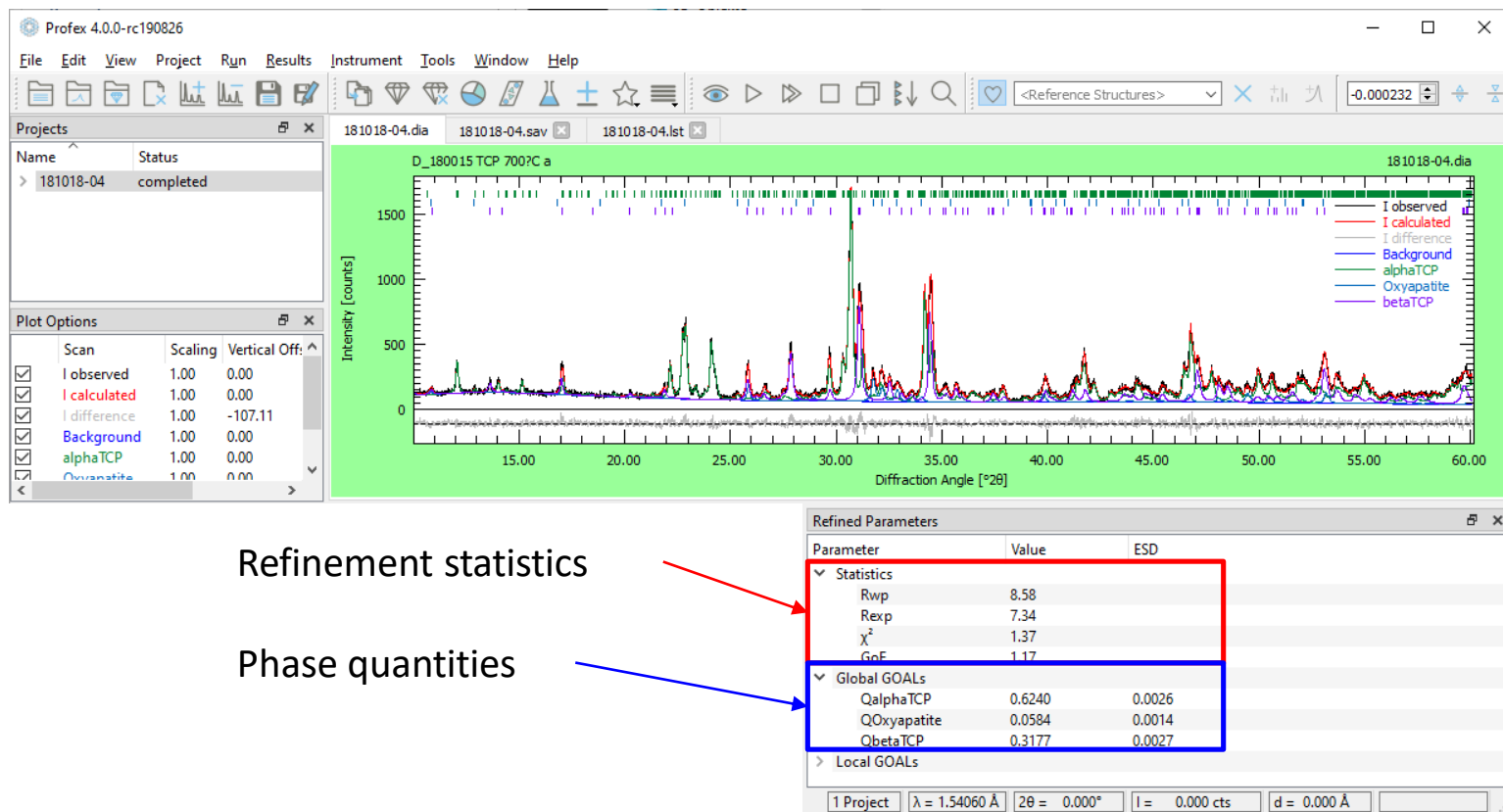
34 sum=alphaTCP+Oxyapatite+betaTCP
35
36 QalphaTCP=alphaTCP/sum
37 QOxyapatite=Oxyapatite/sum
38 QbetaTCP=betaTCP/sum
39
40 GOAL[1]=QalphaTCP
41 GOAL[2]=QOxyapatite
42 GOAL[3]=QbetaTCP
  
```

Text to the right of the screenshot states: "Phase quantification is updated automatically:"

$$sum = \sum GEWICHT$$

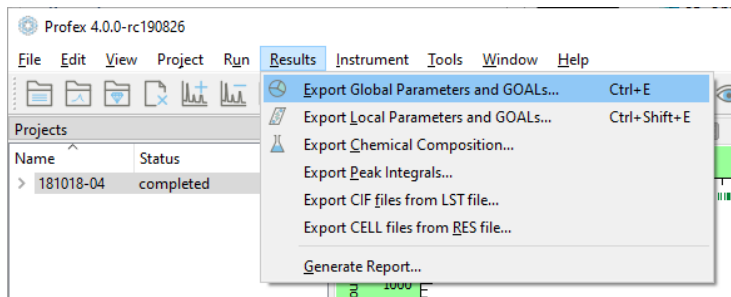
$$Q_{Phase} = \frac{GEWICHT_{Phase}}{sum}$$

Example 2: Favorites / Phase quantification



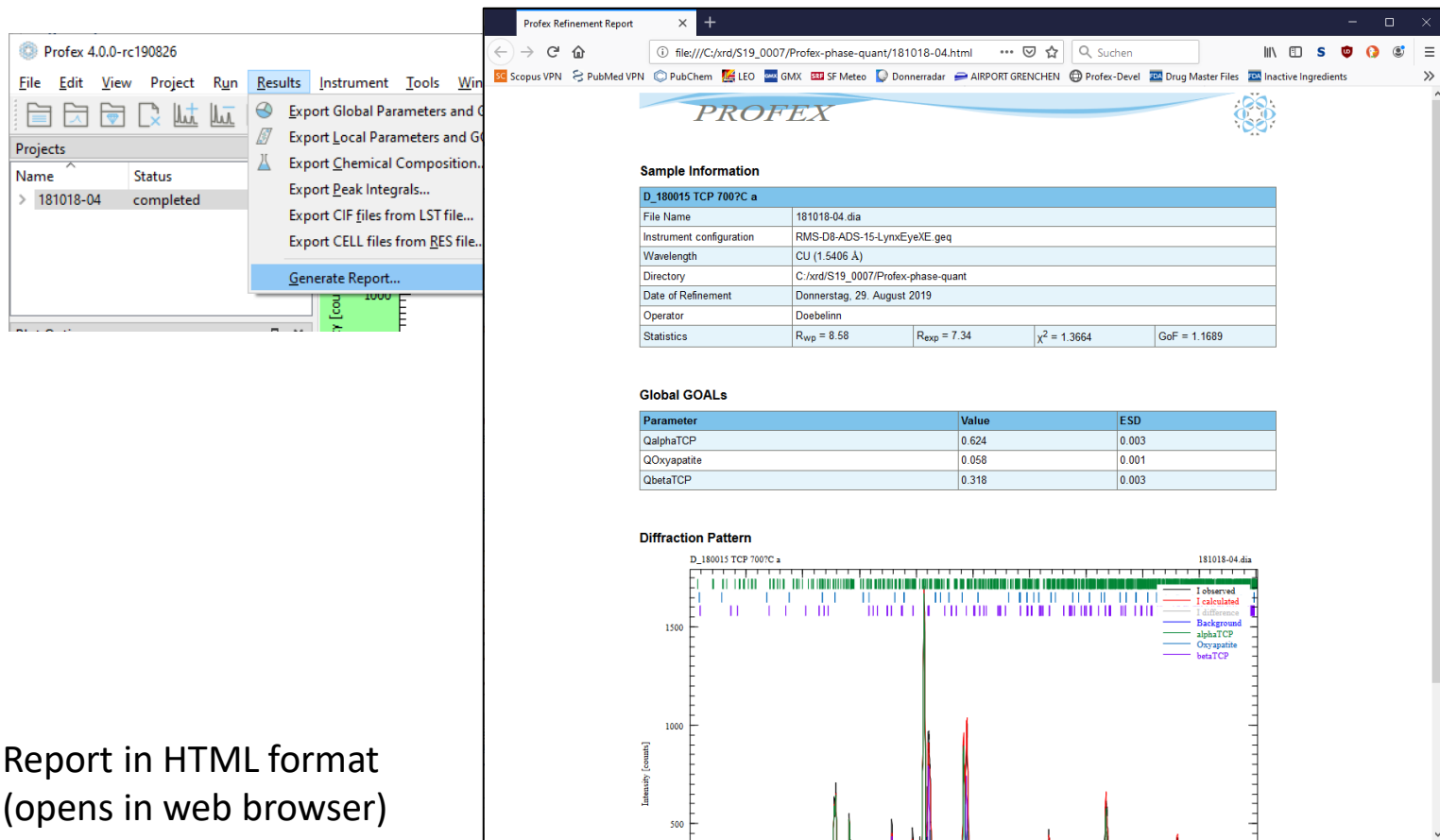
If necessary: Release / fix parameters in STR files → Repeat refinement

Example 2: Exporting Results



File	Sample	Sample ID	Parameter, C Value	ESD
C:/xrd/S19_C181018-04	D_180015 TC QalphaTCP	D_180015 TC QalphaTCP	0.624	0.0026
C:/xrd/S19_C181018-04	D_180015 TC QOxyapatite	D_180015 TC QOxyapatite	0.0584	0.0014
C:/xrd/S19_C181018-04	D_180015 TC QbetaTCP	D_180015 TC QbetaTCP	0.3177	0.0027
C:/xrd/S19_C181018-04	D_180015 TC Rwp	D_180015 TC Rwp	8.58	
C:/xrd/S19_C181018-04	D_180015 TC Rexp	D_180015 TC Rexp	7.34	
C:/xrd/S19_C181018-04	D_180015 TC Chi2	D_180015 TC Chi2	1.3664	
C:/xrd/S19_C181018-04	D_180015 TC GOF	D_180015 TC GOF	1.1689	

Example 2: Exporting Results



The image shows two windows. On the left is the Profex 4.0.0-rc190826 application window. The 'Results' menu is open, and 'Generate Report...' is highlighted. The 'Projects' list shows a project named '181018-04' with a status of 'completed'. On the right is a web browser window displaying the 'Profex Refinement Report' in HTML format. The report includes sample information, global goals, and a diffraction pattern plot.

Sample Information

D_180015 TCP 700?C a				
File Name	181018-04.dia			
Instrument configuration	RMS-D8-ADS-15-LynxEyeXE.geq			
Wavelength	Cu (1.5406 Å)			
Directory	C:/xrd/S19_0007/Profex-phase-quant			
Date of Refinement	Donnerstag, 29. August 2019			
Operator	Doebelinn			
Statistics	$R_{wp} = 8.58$	$R_{exp} = 7.34$	$\chi^2 = 1.3664$	GoF = 1.1689

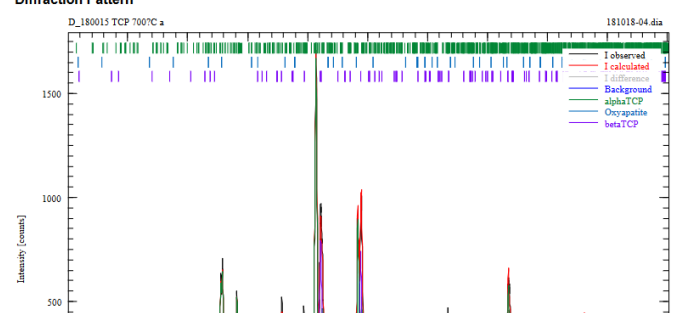
Global GOALS

Parameter	Value	ESD
QalphaTCP	0.624	0.003
QOxyapatite	0.058	0.001
QbetaTCP	0.318	0.003

Diffraction Pattern

D_180015 TCP 700?C a

181018-04.dia



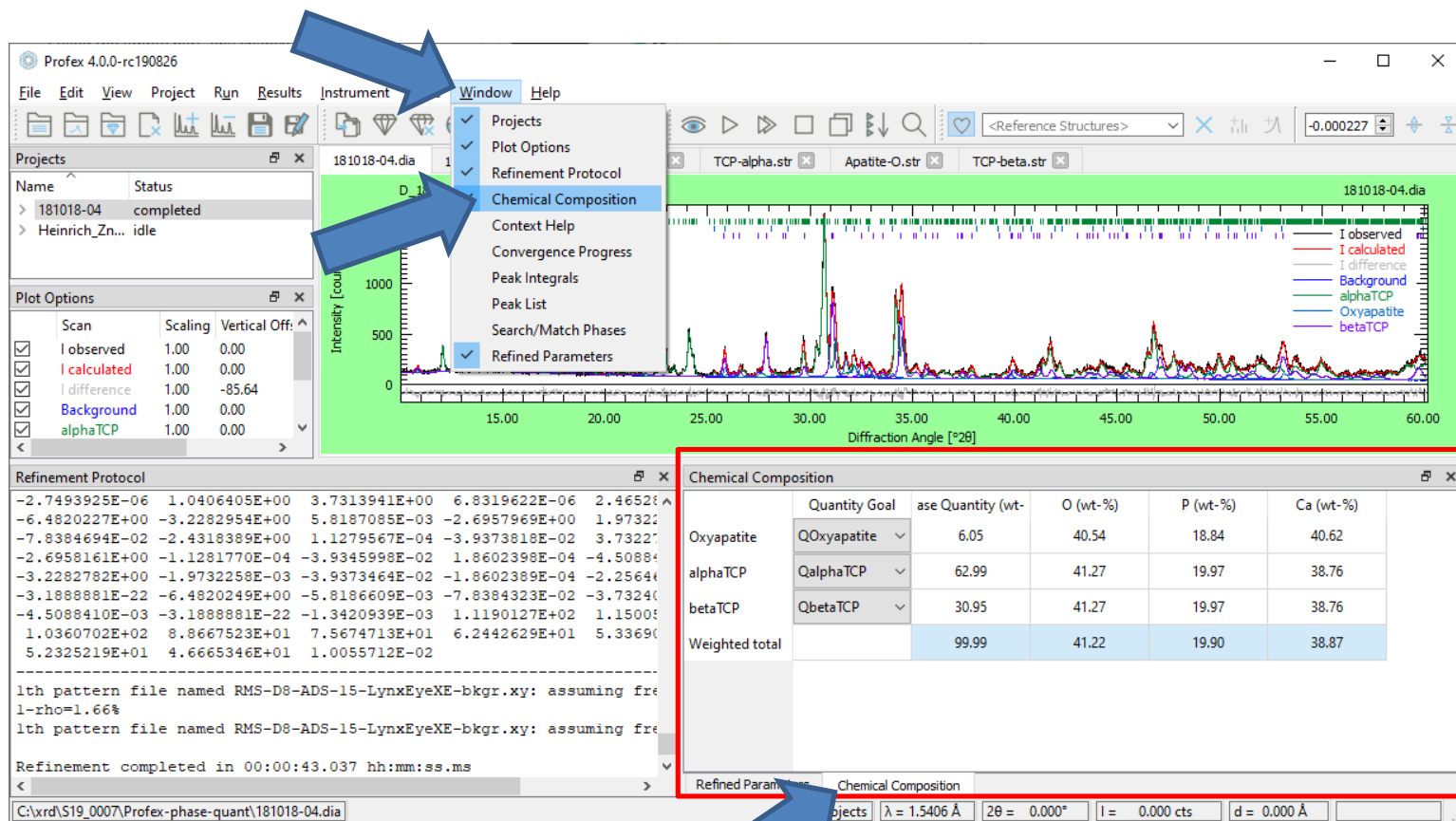
Intensity [counts]

Legend:

- I observed
- I calculated
- I difference
- Background
- alphaTCP
- Oxyapatite
- betaTCP

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

Preferences

- General
- Text Editors
- Graphs
 - Appearance
 - Fonts
 - Scan Styles
 - Print and Export
- BGMN
 - Backend Configuration
 - Repositories
 - Peak Detection
 - Search-Match
 - Reference Structures
 - Favorites
 - Refinement Limits
 - GOAL Management
 - Summary Tables
 - Refinement Report
 - Fullprof.2k
 - Chemical Composition**
 - Text Blocks

Chemical Composition

Calculate composition in:

- Oxides by weight-%
- Elements by weight-%
- Elements by atomic-%
- Oxides by weight-%

	Element	Oxide	
1	H	H2O	18.0152
2	He	He	4.0026
3	Li	Li2O	29.8814
4	Be	BeO	25.0116
5	B	B2O3	69.6202
6	C	CO2	44.0095
7	N	N	14.0067
8	O	O	15.9994
9	F	F	18.9984
10	Ne	Ne	20.1797

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

Chemical Composition

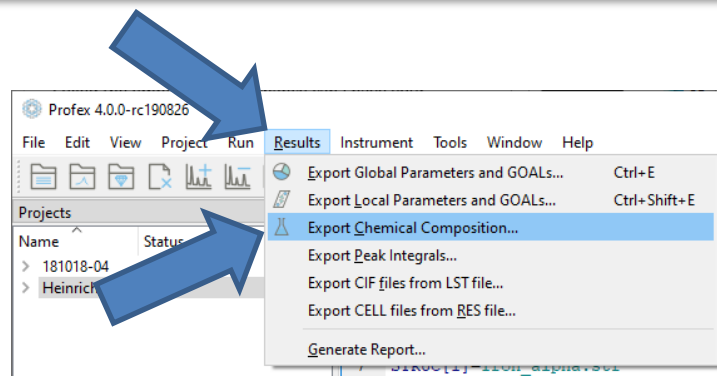
	Quantity Goal	Phase Quantity (wt-%)	O (atm-%)	P (atm-%)	Ca (atm-%)
Oxyapatite	QOxyapatite	6.05	60.98	14.63	24.39
alphaTCP	QalphaTCP	62.99	61.54	15.38	23.08
betaTCP	QbetaTCP	30.95	61.54	15.38	23.08
Weighted total		-	-	-	-

Chemical Composition

	Quantity Goal	Phase Quantity (wt-%)	P2O5 (wt-%)	CaO (wt-%)
Oxyapatite	QOxyapatite	6.05	43.16	56.84
alphaTCP	QalphaTCP	62.99	45.76	54.24
betaTCP	QbetaTCP	30.95	45.76	54.24
Weighted total		99.99	45.60	54.39

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

