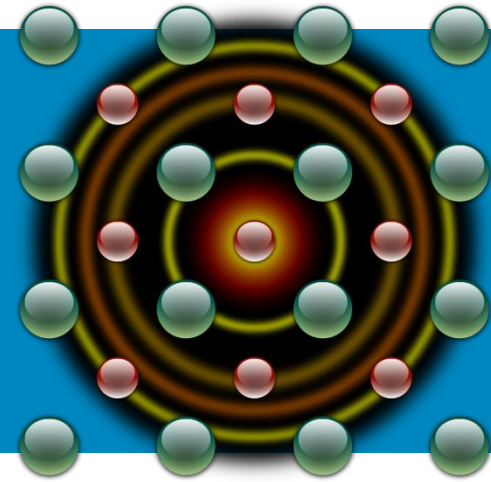


Lesson 6

Profex

Graphical User Interface for BGMN
and Fullprof



Nicola Döbelin
RMS Foundation, Bettlach, Switzerland

Background Information

Developer: Nicola Döbelin (private)

License: GPL v2 or later (open source)

Founded in: 2003

Platforms: Windows XP / Vista / 7 / 8 / 10
Linux
Mac OS X 10.7 -10.11 (64bit)

Rietveld Backends: BGMN, Fullprof.2k

Website: <http://profex.doebelin.org>

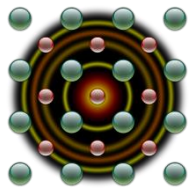
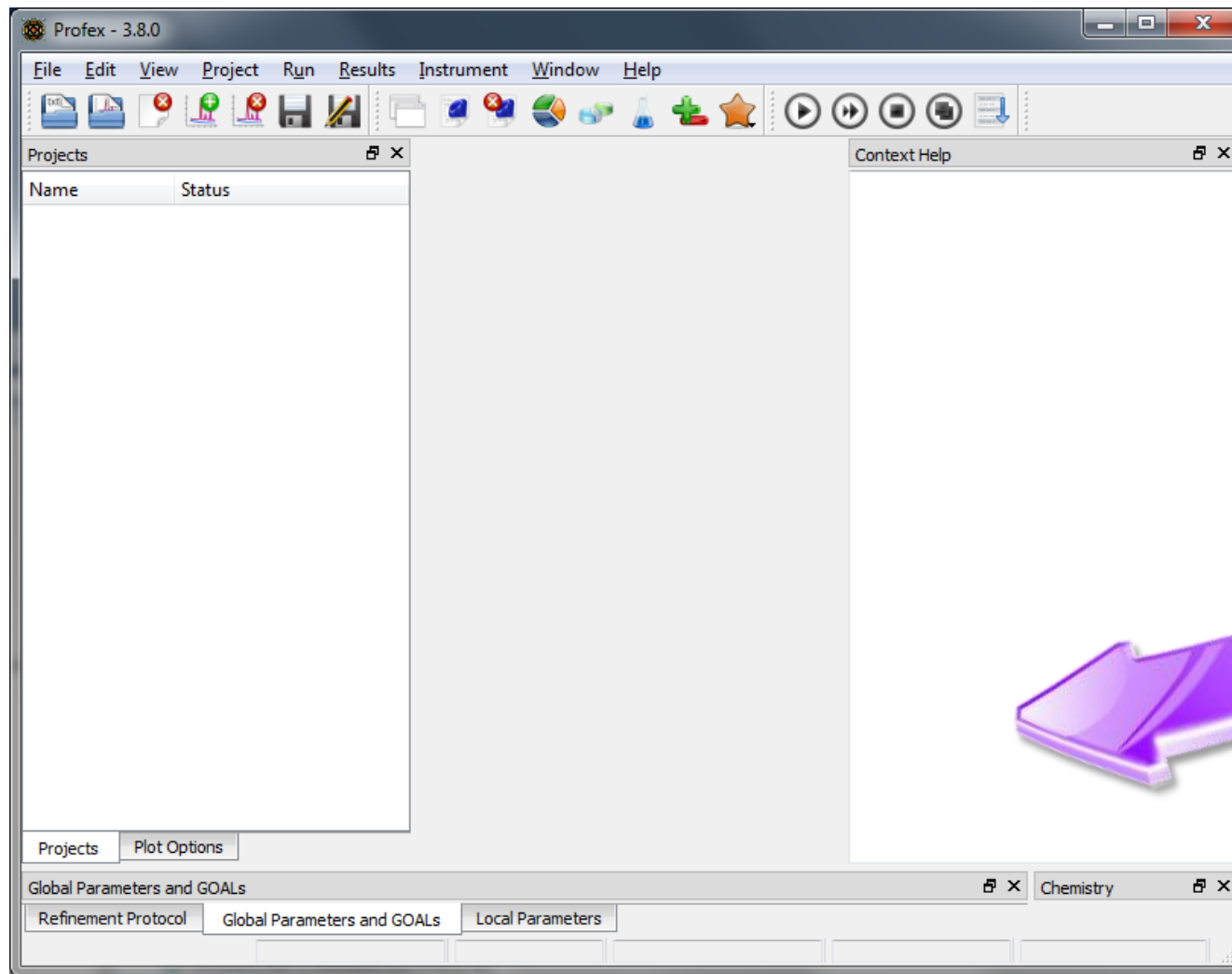
Current stable version: 3.10.1

History

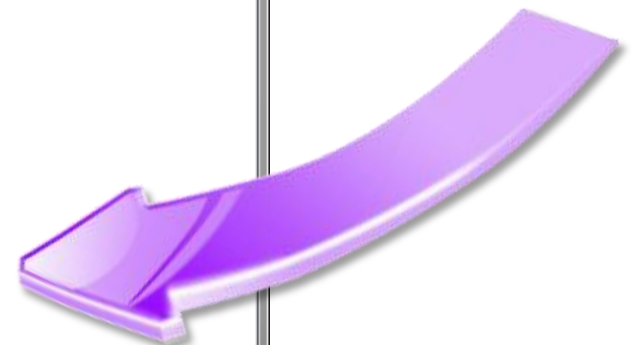
- 2003: Start of development as an alternative GUI for Fullprof.2k
For personal use only (my PhD)
Linux only
- 2006: Major rewrite
Support for Windows
- 2012: Support for BGMN Rietveld Backend added
- 2014: Support for Mac OS X



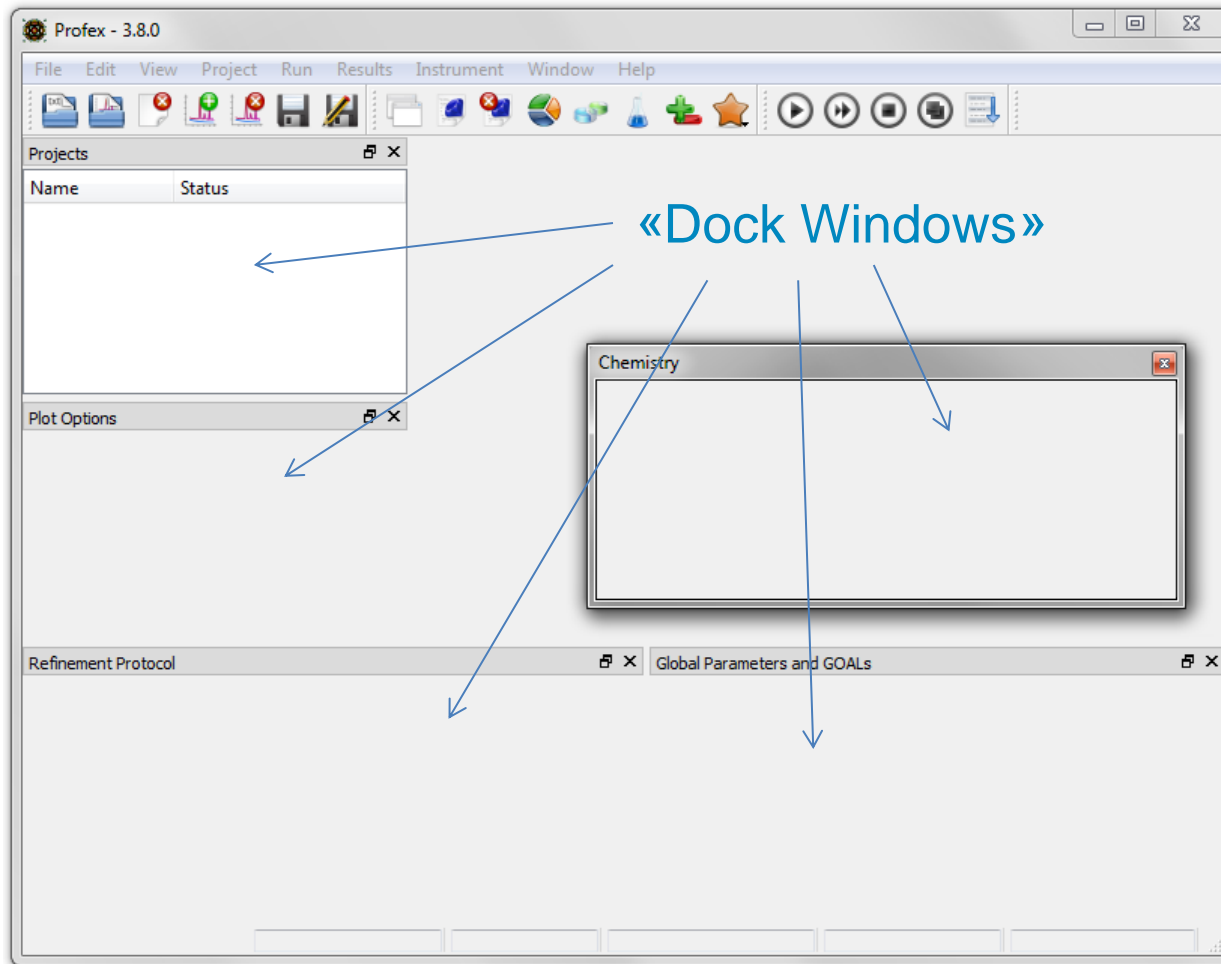
First Use



Profex



First Use



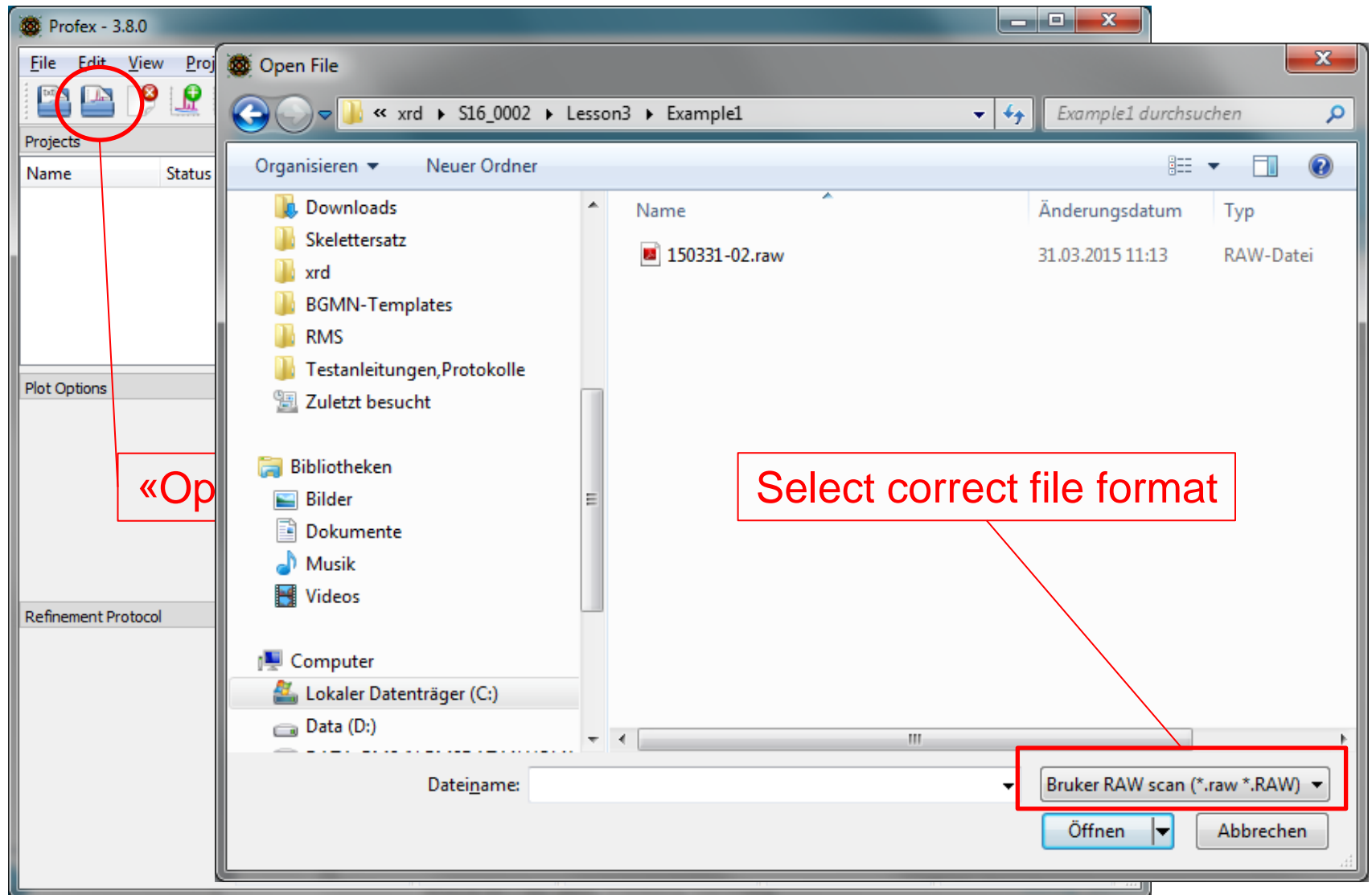
Can be re-arranged
(drag & drop)

Stacked

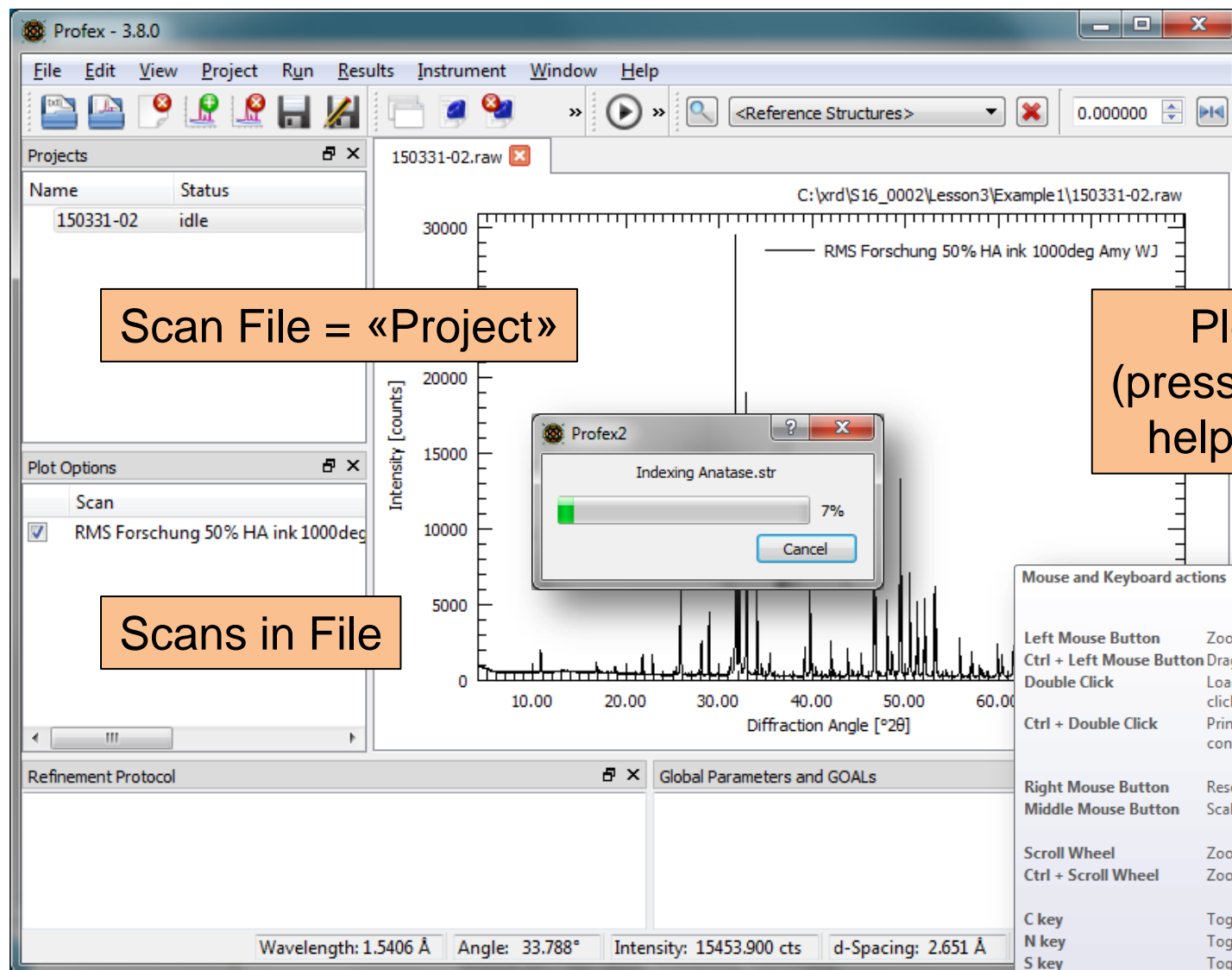
Floating

Closed
(opened from
«Window» menu)

Load Scan File



First Use: Example 1



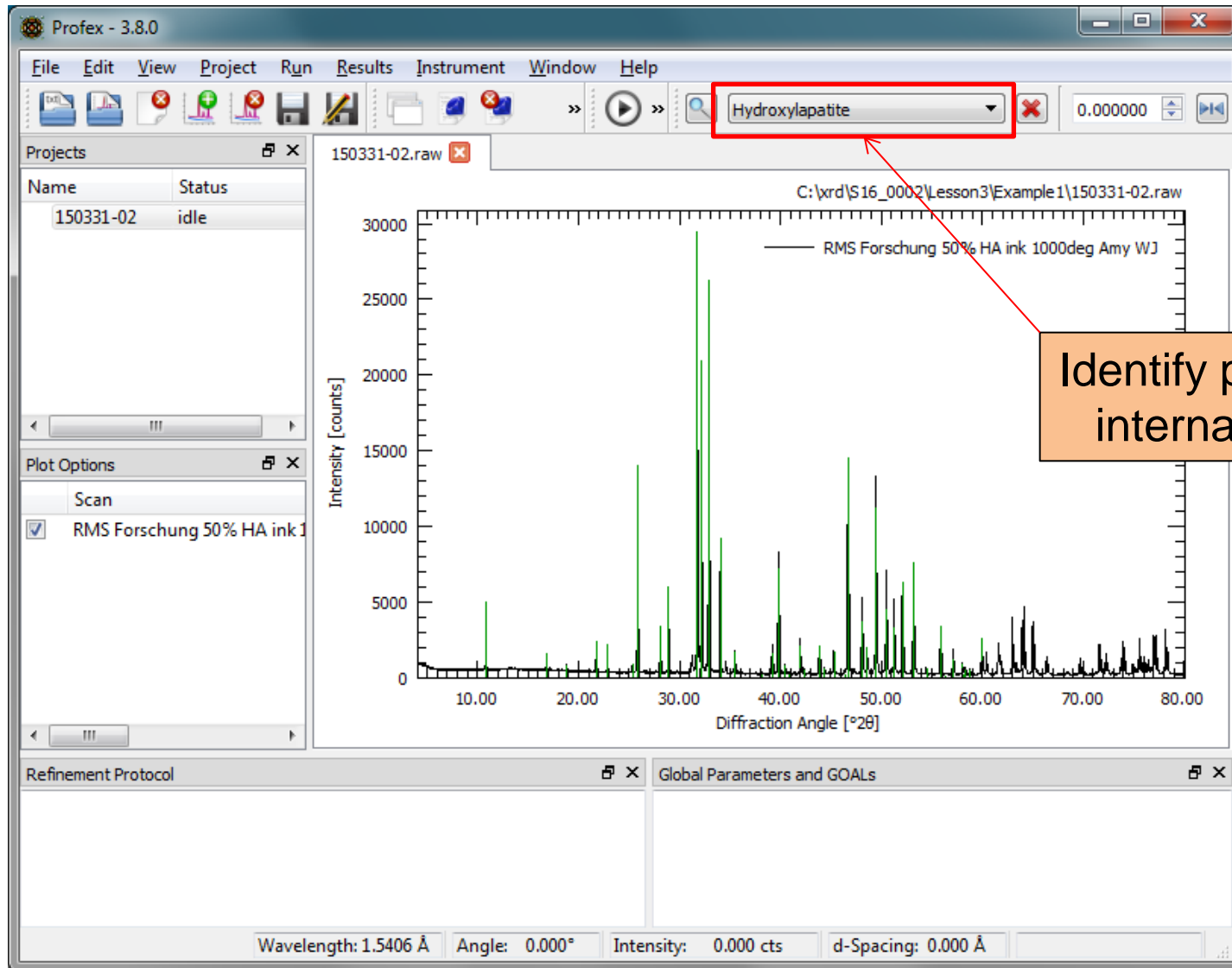
Scan File = «Project»

Scans in File

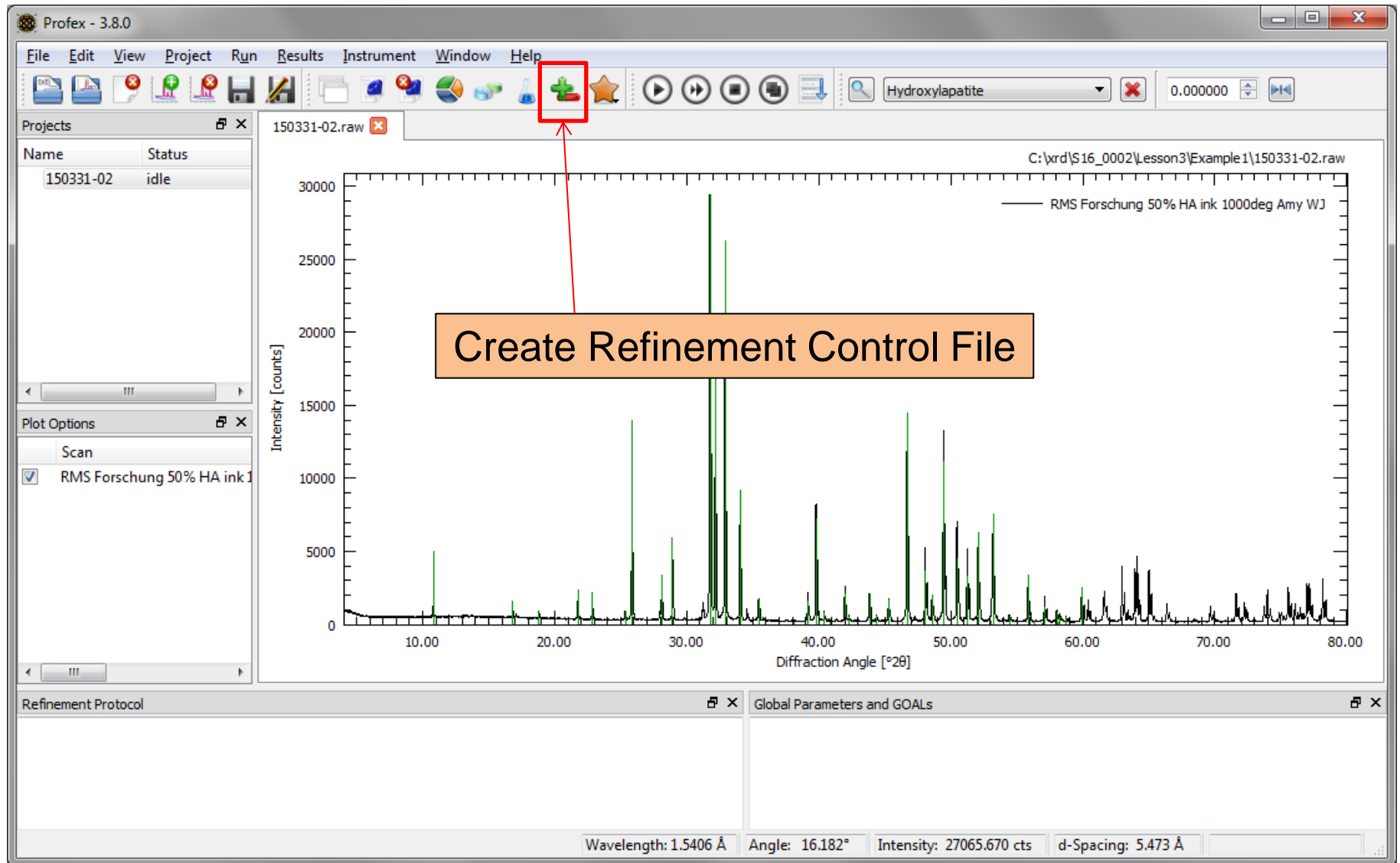
Plot area
(press «shift» for
help window)

Mouse and Keyboard actions	
Left Mouse Button	Zoom
Ctrl + Left Mouse Button	Drag view
Double Click	Load reference structure with strongest peak at click position
Ctrl + Double Click	Print current coordinates to refinement protocol console
Right Mouse Button	Reset zoom
Middle Mouse Button	Scale intensity of reference lines
Scroll Wheel	Zoom horizontally
Ctrl + Scroll Wheel	Zoom vertically
C key	Toggle cross hair cursor on / off
N key	Toggle noise cursor on / off
S key	Toggle spectral line cursor on / off

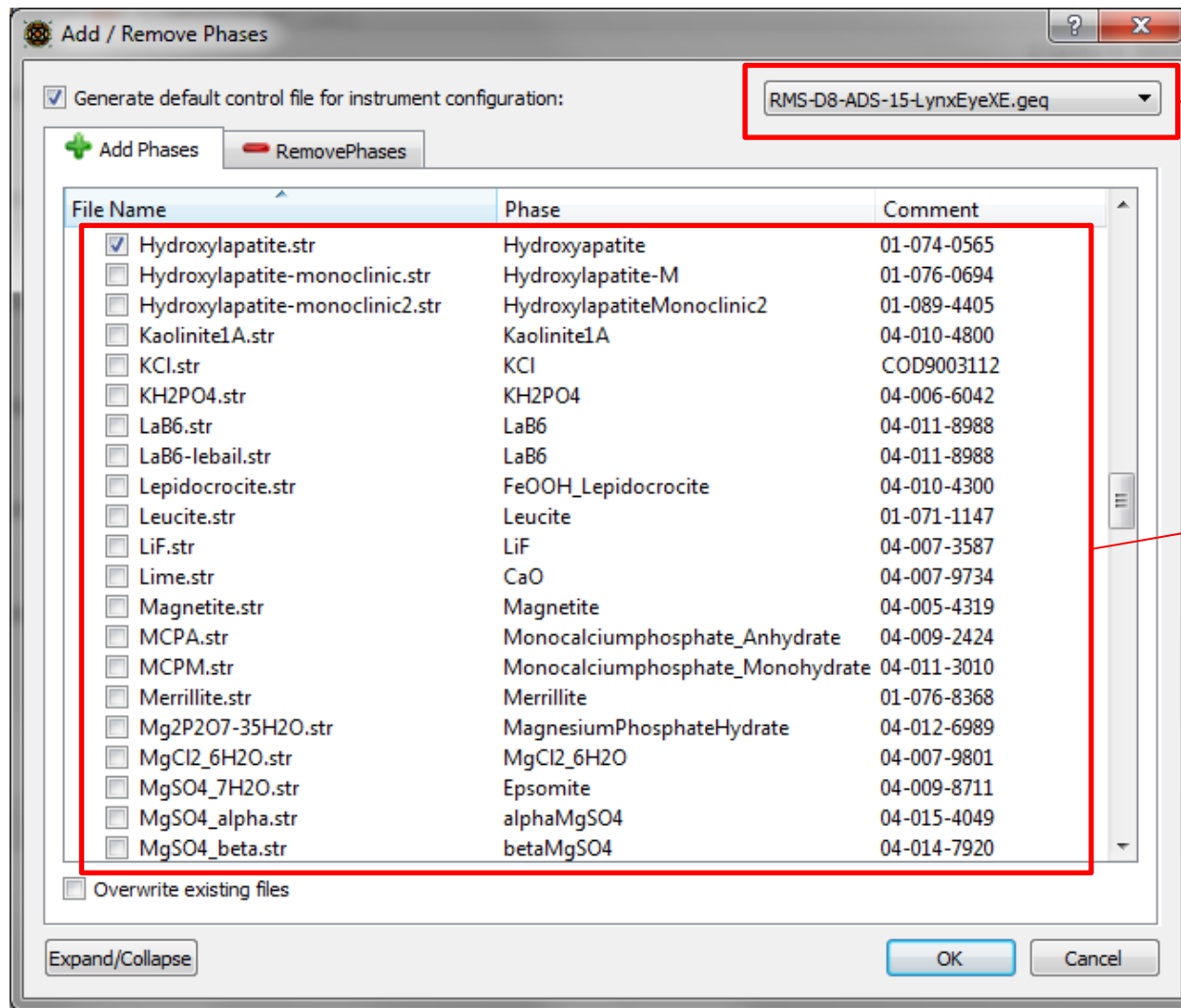
First Use: Example 1



First Use: Example 1



First Use: Example 1



Choose correct instrument configuration

Select phases (HAp is pre-selected)

First Use: Example 1

The screenshot shows the Profex 3.8.0 software interface. The main window displays a project named '150331-02' with a status of 'idle'. The 'Plot Options' section is set to 'Scan'. The main text area contains the following content:

```
% SampleID: RMS Forschung 50% HA ink 1000deg Amy WJ
% Theoretical instrumental function
VERZERR=RMS-D8-ADS-15-LynxEyeXE.geq
% Wavelength
LAMBDA=CU
% Phases
STRUC[1]=Hydroxylapatite.str
% Measured background
UNT=RMS-D8-ADS-15-LynxEyeXE-bkgr.xy
% Measured data
VAL[1]=150331-02.xy
% Minimum Angle (2theta)
WMIN=10
% Maximum Angle (2theta)
WMAX=60
% Result list output
LIST=150331-02.lst
% Peak list output
OUTPUT=150331-02.par
% Diagram output
DIAGRAMM=150331-02.dia
% Global parameters for zero point and sample displacement
EPS1=0
PARAM[1]=EPS2=0_-0.01^0.01
EPS3=0
alpha3ratio=0.020
betaratio=0.0
NTHREADS=8
PROTOKOLL=Y
SAVE=N

sum=HAp
GOAL f1=HAn/sim
```

A red box highlights the '150331-02.sav*' file in the project window. A red arrow points from this box to a callout box containing the text: "New BGMN Refinement Control File was generated".

At the bottom of the interface, the status bar shows: Wavelength: 1.5406 Å, Angle: 0.000°, Intensity: 0.000 cts, d-Spacing: 0.000 Å, Line 0, Column 0.

First Use: Example 1

The screenshot shows the Profex 3.8.0 software interface. The main window displays a list of parameters for a refinement process, including sample information, theoretical instrumental function, measured data, and refinement options. The 'Run' button (a play icon) in the toolbar is highlighted with a red box, and a red arrow points to it from a text box that says "Run the refinement".

Projects: 150331-02.raw, 150331-02.sav*

Name	Status
150331-02	idle

Plot Options: Scan, RMS Forschung 50% HA ink 1

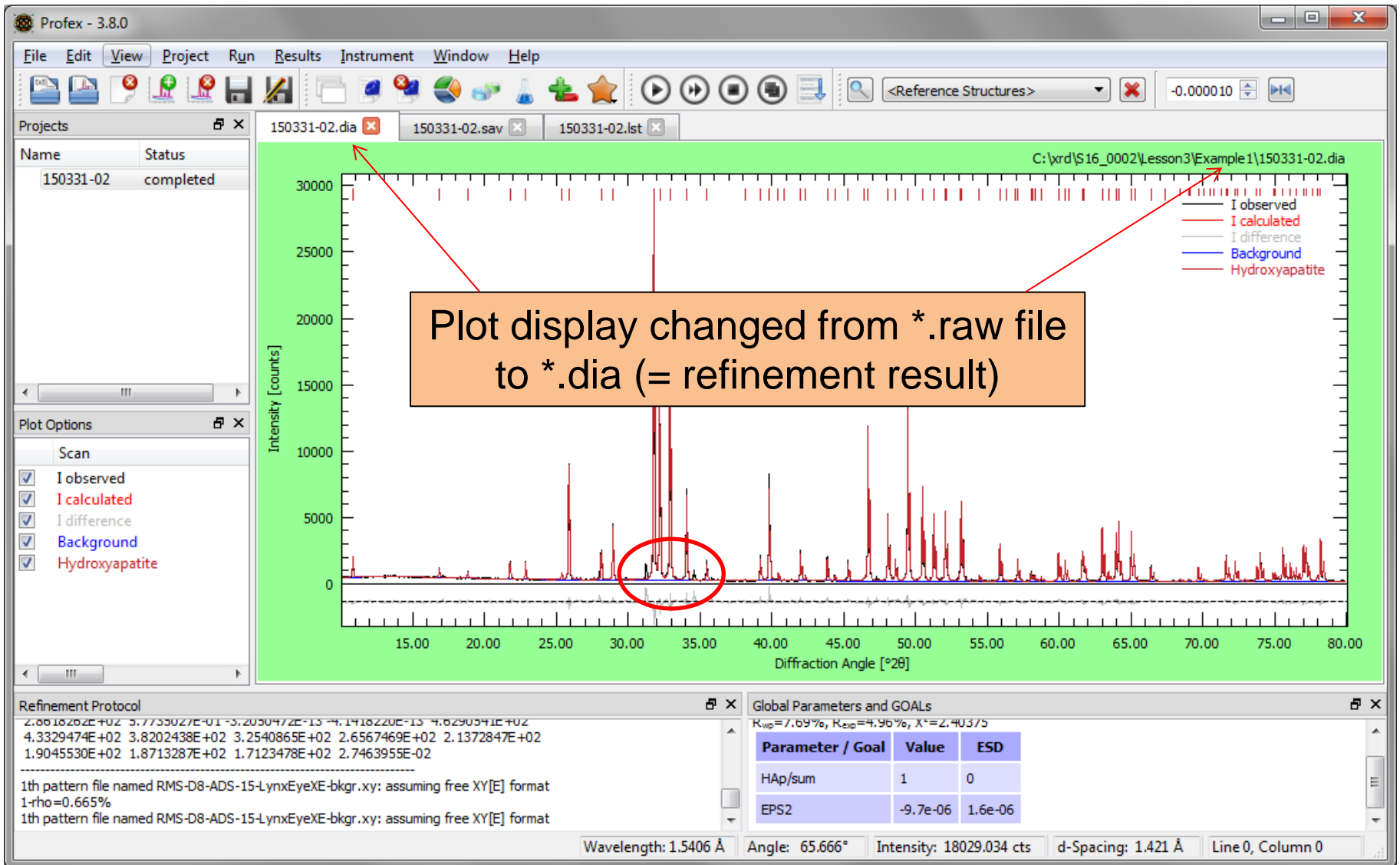
```
% SampleID: RMS Forschung 50% HA ink 1000deg Amy WJ
% Theoretical instrumental function
VERZERR=RMS-D8-ADS-15-LynxEyeXE.geq
% Wavelength
LAMBDA=CU
% Phases
STRUC[1]=Hydroxylapatite.str
% Measured background
UNT=RMS-D8-ADS-15-LynxEyeXE-bkgr.xy
% Measured data
VAL[1]=150331-02.xy
% Minimum Angle (2theta)
WMIN=10
% Maximum Angle (2theta)
WMAX=60
% Result list output
LIST=150331-02.lst
% Peak list output
OUTPUT=150331-02.par
% Diagram output
DIAGRAMM=150331-02.dia
% Global parameters for zero point and sample displacement
EPS1=0
PARAM[1]=EPS2=0_-0.01^0.01
EPS3=0
alpha3ratio=0.020
betaratio=0.0
NTHREADS=8
PROTOKOLL=Y
SAVE=N

sum=HAp
GOAL f1=HAn/sim
```

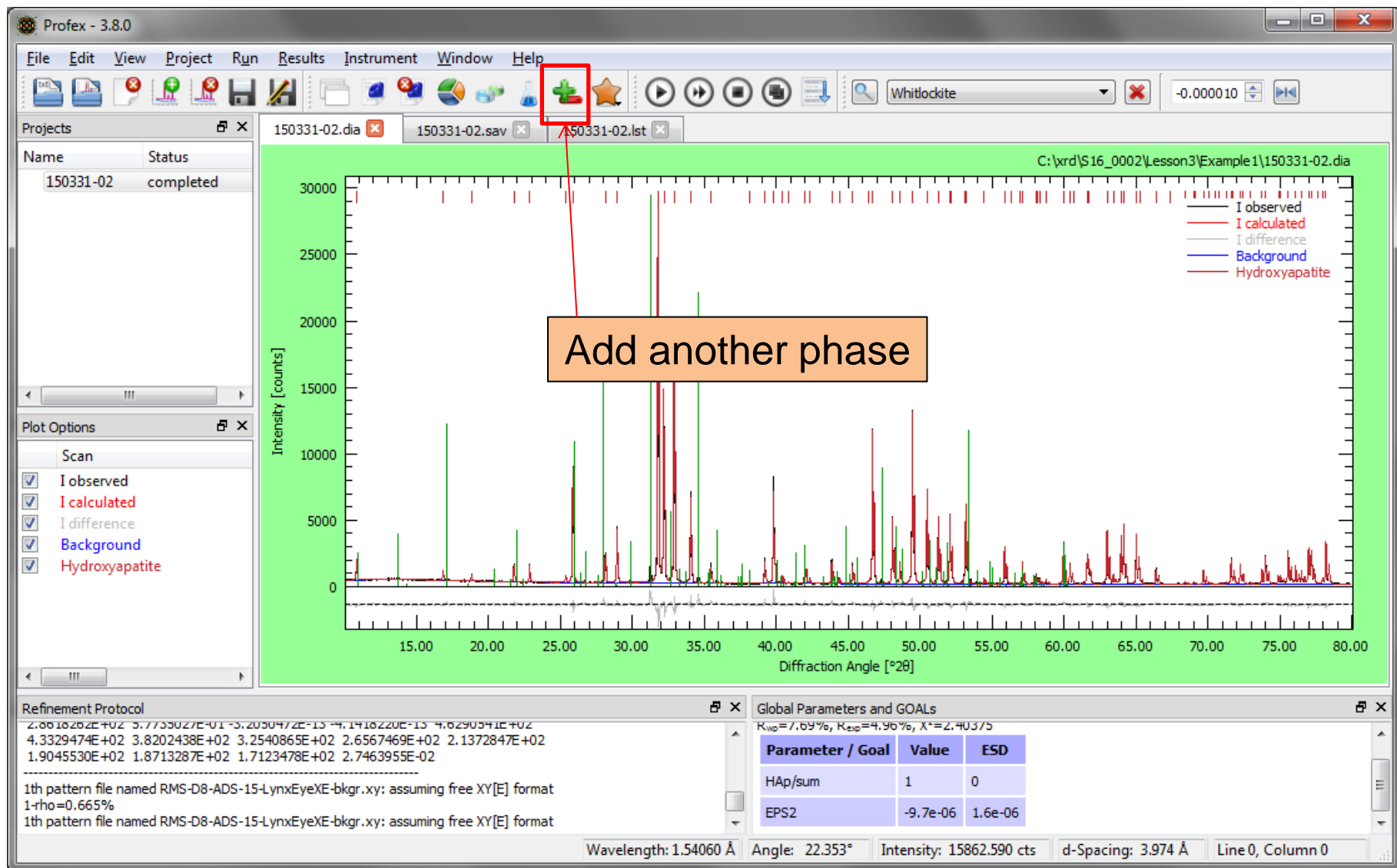
Refinement Protocol: Global Parameters and GOALS

Wavelength: 1.5406 Å Angle: 0.000° Intensity: 0.000 cts d-Spacing: 0.000 Å Line 0, Column 0

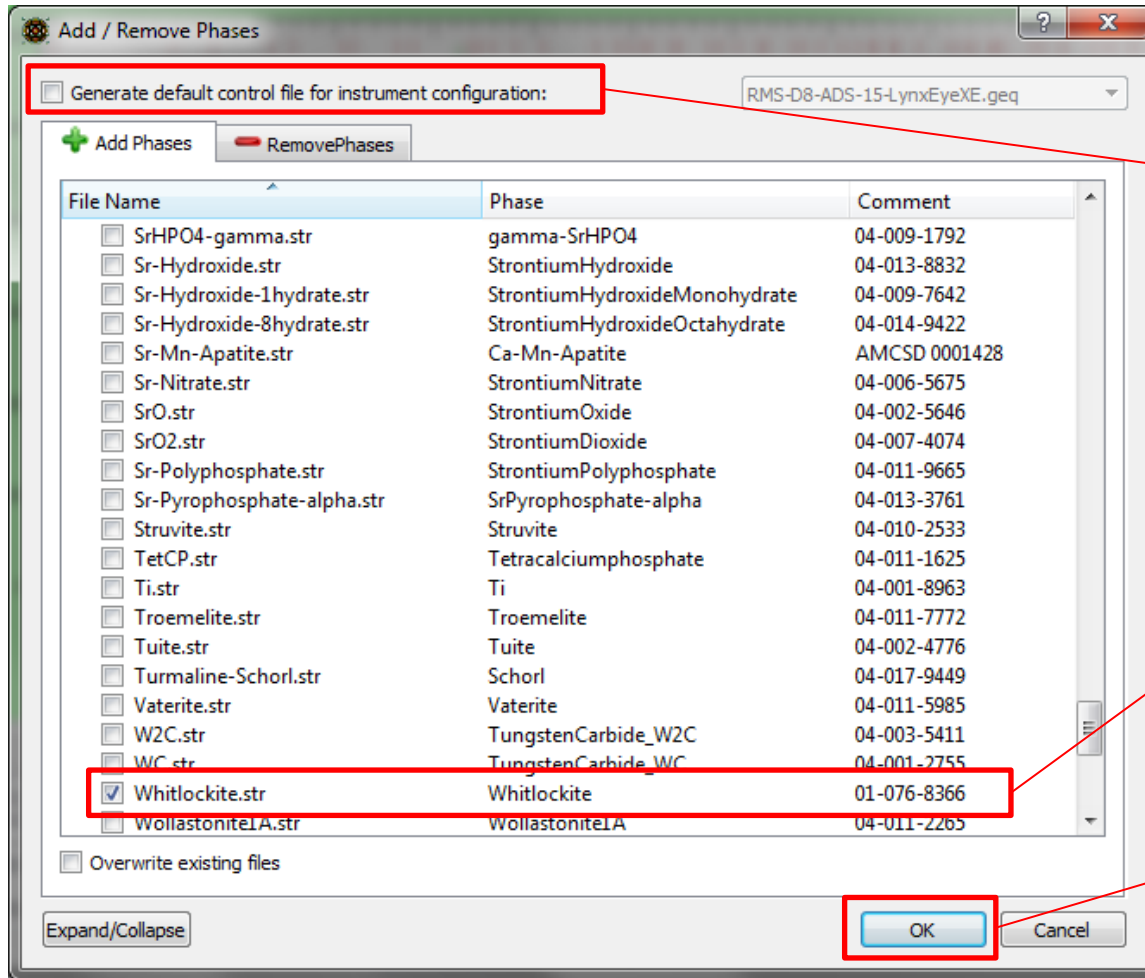
First Use: Example 1



First Use: Example 1



First Use: Example 1

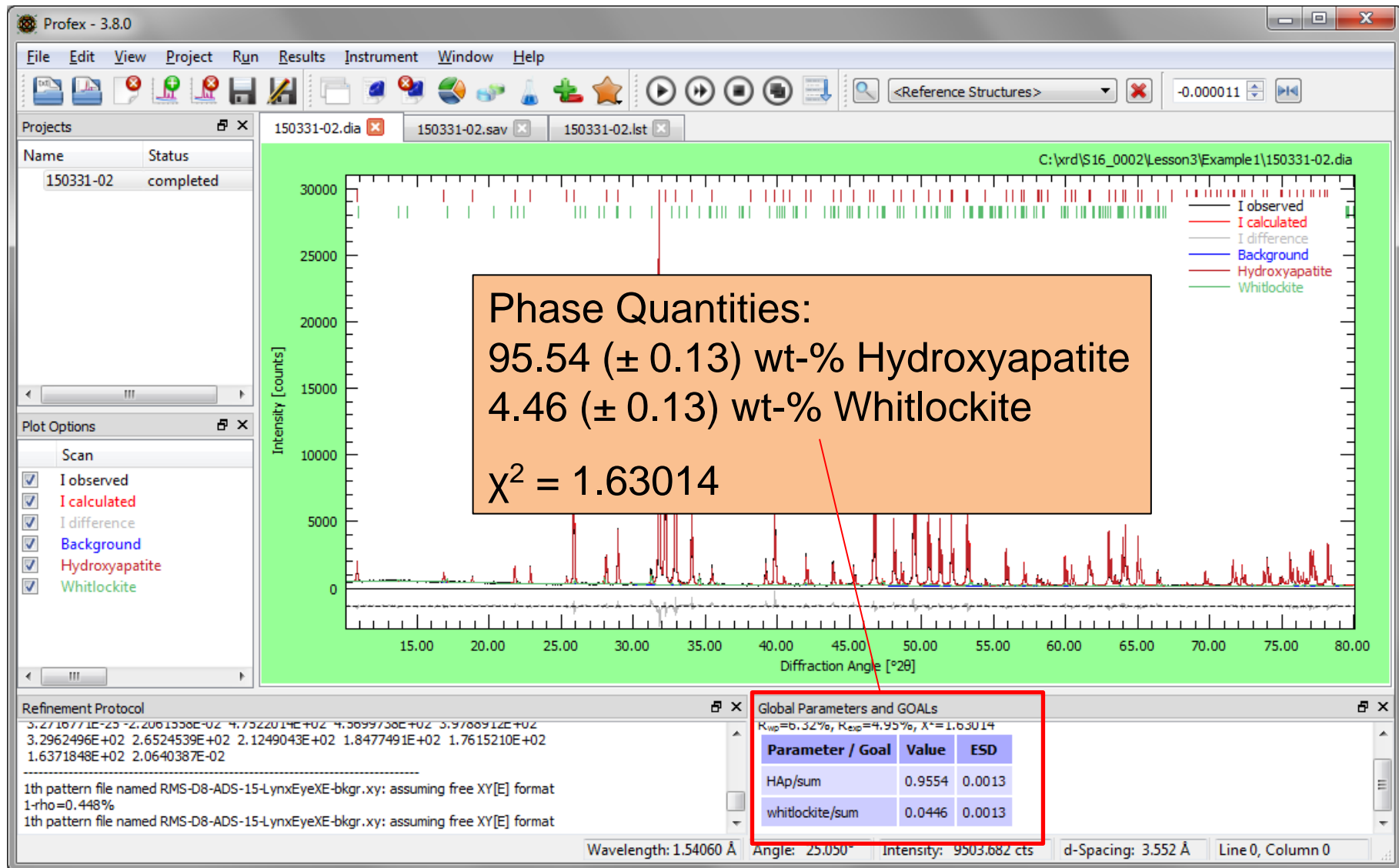


Control file already exists, **don't** generate a new default file

Select Whitlockite

Click «OK» and re-run the refinement

First Use: Example 1



First Use: Example 1

Profex - 3.8.0

File Edit View Project Run Results Instrument Window Help

Projects: 150331-02.dia, 150331-02.sav, 150331-02.lst

Name Status
150331-02 completed

Rietveld refinement to file(s) 150331-02.xy
BGMN version 4.2.22, 5716 measured points, 364 peaks, 52 parameters
Start: Wed Feb 24 10:50:11 2016; End: Wed Feb 24 10:50:17 2016
34 iteration steps

Rp=5.69% Rpb=9.35% R=5.68% Rwp=6.32% Rexp=4.95%
Durbin-Watson d=0.87
1-rho=0.448%

Global parameters and GOALS

HAp/sum=0.9554+-0.0013
whitlockite/sum=0.0446+-0.0013
EPS2=-0.0000113+-0.0000013

Local parameters and GOALS for phase Hydroxyapatite

SpacegroupNo=176
HermannMauguin=P6_3/m
XrayDensity=3.152
Rphase=5.77%
UNIT=NM
A=0.9421883+-0.0000024
C=0.6884401+-0.0000022
GrainSize(0,0,1)=315.6+-4.3
GrainSize(1,0,0)=323.7+-2.7
GEWICHT=SPHAR4, MeanValue(GEWICHT)=0.347882
B1=ANISOLIN, MeanValue(B1)=0.00132246, sqrt3(det(B1))=0.00132231
Atomic positions for phase Hydroxyapatite

4 0.3333 0.6667 0.0015 E=(CA(1.0000))
6 0.2468 0.9934 0.2500 E=(CA(1.0000))
6 0.3987 0.3685 0.2500 F=(P(1.0000))

Plot Options
Scan
 I observed
 I calculated
 I difference
 Background
 Hydroxyapatite
 Whitlockite

Refinement Protocol
3.2716771E+23 -2.2061550E+02 4.7522014E+02 4.3699738E+02 3.9788912E+02
3.2962496E+02 2.6524539E+02 2.1249043E+02 1.8477491E+02 1.7615210E+02
1.6371848E+02 2.0640387E-02

1th pattern file named RMS-D8-ADS-15-LynxEyeXE-bkgr.xy: assuming free XY[E] format
1-rho=0.448%
1th pattern file named RMS-D8-ADS-15-LynxEyeXE-bkgr.xy: assuming free XY[E] format

Global Parameters and GOALS
Kwp=6.32%, Rexp=4.95%, X*=1.63014

Parameter / Goal	Value	ESD
HAp/sum	0.9554	0.0013
whitlockite/sum	0.0446	0.0013

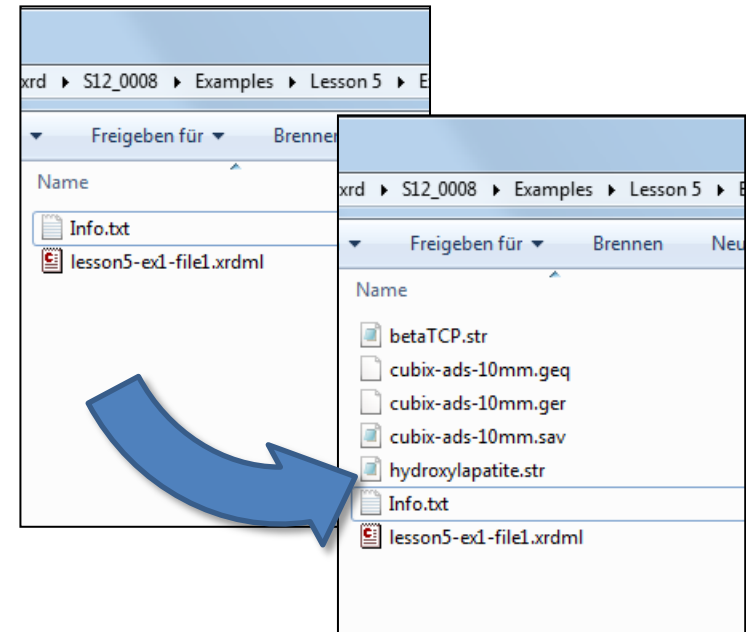
Wavelength: 1.54060 Å Angle: 0.000° Intensity: 0.000 cts d-Spacing: 0.000 Å Line 0, Column 0

*.lst file with detailed refinement results opened automatically

Features of Profex (I)

What Profex does in the background:

- Generate a control file
- Copy all selected structure files from local DB to location of scan file
- Copy instrument configuration file from local DB to location of scan file
- Adjust file names in control file
- Converts Raw Scan format to XY format for BGMN
- Convert file formats (Windowx ↔ Unix/Mac)
- Adjusts GOALs for phase quantification



Features of Profex (II)

```
lesson3-ex1-file1.dia lesson3-ex1-file1.sav lesson3-ex1-file1.lst
% Theoretical instrumental function
VERZERR=cubix-ads-10mm.geq
% Wavelength
LAMBDA=CU
% Polarization (CuKa with Graphite monochromator)
POL=sqr(cos(26.6*pi/180))
pi=2*acos(0)
% Phases
STRUC[1]=betaTCP.str
STRUC[2]=hydroxylapatite.str
% Measured data
VAL[1]=lesson3-ex1-file1.xy
% Minimum Angle (2theta)
% WMIN=10
% Maximum Angle (2theta)
% WMAX=60
% Result list output
LIST=lesson3-ex1-file1.lst
% Peak list output
OUTPUT=lesson3-ex1-file1.par
% Diagram output
DIAGRAMM=lesson3-ex1-file1.dia
% Global parameters for zero point and sample displacement
EPS1=0
PARAM[1]=EPS2=0_-0.01^0.01
PARAM[2]=Bglobal=0_0^0.01
alpha3ratio=0.02
betaratio=0
NTHREADS=8
PROTOKOLL=Y

GOAL[1]=betaTCP/(betaTCP+hap)
GOAL[2]=hap/(betaTCP+hap)
```

Handled by Profex:

Instrument config file

Structure files

Conversion of raw scan
XRDML → XY

Automatic file names
of output files

GOALs for phase
quantification

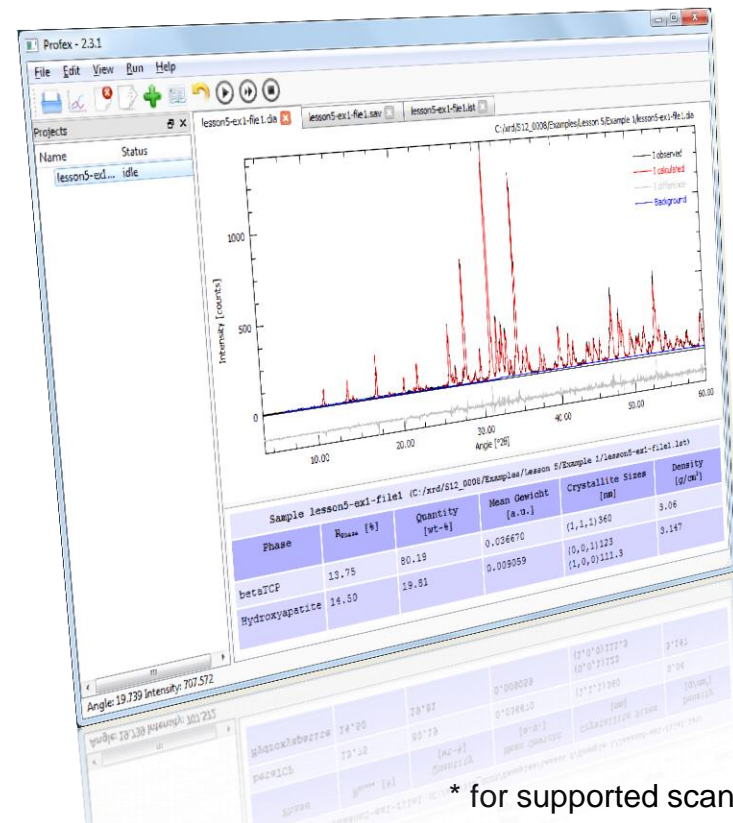
Features of Profex (III)

With Profex:

1. Load scan file
2. Use «Append phase» dialog to select phases, instrument, and generate control file
3. Run refinement

No need to:

- Copy structure / device files
- Change any file names
- Convert scan files*



* for supported scan file formats

Features of Profex (IV)

Advantages:

- Very efficient workflow for many use cases
- Automatic / batch refinements
- Easier learning curve

Disadvantages:

- Restrictions in choice of file names: Do not force Profex to use different file names than the auto-generated ones



Optimizing the Refinement

The screenshot shows the Profex 3.8.0 interface. The main text area contains the following text:

```
% SampleID: RMS Forschung 50% HA ink 1000deg Amy WJ
% Theoretical instrumental function
VERZERR=RMS-D8-ADS-15-LynxEyeXE.geq
% Wavelength
LAMBDA=CU
% Phases
STRUC[1]=Hydroxyapatite.str
STRUC[2]=Whitlockite.str
% Measured background
UNT=RMS-D8-ADS-15-LynxEyeXE.geq
% Measured data
VAL[1]=150331-02.xy
% Minimum Angle (2theta)
WMIN=10
% Maximum Angle (2theta)
WMAX=60
% Result list output
LIST=150331-02.lst
% Peak list output
OUTPUT=150331-02.par
% Diagram output
DIAGRAMM=150331-02.dia
% Global parameters for refinement
EPS1=0
PARAM[1]=EPS2=0_-0.001
EPS3=0
alpha3ratio=0.020
betaratio=0.0
NTHREADS=8
PROTOKOLL=Y
SAVE=N
sum=HAp+whitlockite
```

A context menu is open over the line `STRUC[1]=Hydroxyapatite.str`. The menu items are:

- Undo
- Redo (Ctrl+Y)
- Cut (Ctrl+X)
- Copy
- Paste (Ctrl+V)
- Delete
- Select All (Ctrl+A)
- Open file
- Add STRUCOUT file
- Add SimpleSTRUCOUT file
- Add RESOUT file
- Add FCFOU file
- Add PDBOUT file

An orange callout box contains the text: "Right-click on line «STRUC[1]=Hydroxyapatite.str» And select «Open File»". Red arrows point from the text in the callout box to the right-click location and the "Open file" menu item.

The bottom panel shows the Refinement Protocol and Global Parameters and GOALS:

Refinement Protocol:

```
3.2716771E+25 -2.2061330E+02 4.7522014E+02 4.3699738E+02 3.9788912E+02
3.2962496E+02 2.6524539E+02 2.1249043E+02 1.8477491E+02 1.7615210E+02
1.6371848E+02 2.0640387E-02
```

Global Parameters and GOALS:

Parameter / Goal	Value	ESD
HAp/sum	0.9554	0.0013
whitlockite/sum	0.0446	0.0013

Wavelength: 1.54060 Å Angle: 0.000° Intensity: 0.000 cts d-Spacing: 0.000 Å Line 6, Column 21

Optimizing the Refinement

The screenshot shows the Profex 3.8.0 interface. The 'Projects' panel on the left lists '150331-02' as 'completed'. The main window displays the refinement protocol for Hydroxylapatite. The 'Global Parameters and GOALS' panel at the bottom right shows the following table:

Parameter / Goal	Value	ESD
HAp/sum	0.9554	0.0013
whitlockite/sum	0.0446	0.0013

Two callout boxes provide instructions: 'Alternatively click «Open all Project Structure Files»' points to a button in the toolbar, and 'Opens both structure files' points to the 'Hydroxylapatite.str' and 'Whitlockite.str' files in the project list.

BGMN Control / Structure File Syntax

$X=0$

Parameter X is fixed at the value 0
X is not refined

$PARAM=X=0$

Parameter X is initialized with the value 0
X is released for refinement

$PARAM=X=0_{-1}^{1}$

Parameter X is initialized with the value 0
X is released for refinement
X can vary between -1 and 1

$X=ANISO^{1}$

Parameter X is initialized with the value 0
X is released for anisotropic refinement
X can vary between 0 and 1
(e.g. size of the crystallites)

Optimizing the Refinement

Profex - 3.8.0

File Edit View Project Run Results Instrument Window Help

Projects: 150331-02.dia, 150331-02.sav, 150331-02.lst, Hydroxylapatite.str, Whitlockite.str

Name Status
150331-02 completed

PHASE=Hydroxyapatite // 01-074-0565
MineralName=Hydroxylapatite //
Formula=Ca5_(PO4)3_(OH) //
SpacegroupNo=176 HermannMauguin=P6_3/m //
PARAM=A=0.9424_0.9330^0.9518 PARAM=C=0.6879_0.6610^0.6948 //
RP=4 k1=0 k2=0
GOAL=GrainSize
GOAL=GrainSize
GOAL:HAp=GEV
E=CA Wyckoff=
E=CA Wyckoff=
E=P Wyckoff=h
E=O Wyckoff=h
E=O Wyckoff=h
E=O Wyckoff=i
E=O(0.5000) W
E=H(0.5000) W

Context Menu:
Undo
Redo Ctrl+Y
Cut Ctrl+X
Copy
Paste Ctrl+V
Delete
Select All Ctrl+A
Refine isotropically
Refine anisotropically
Fix parameter

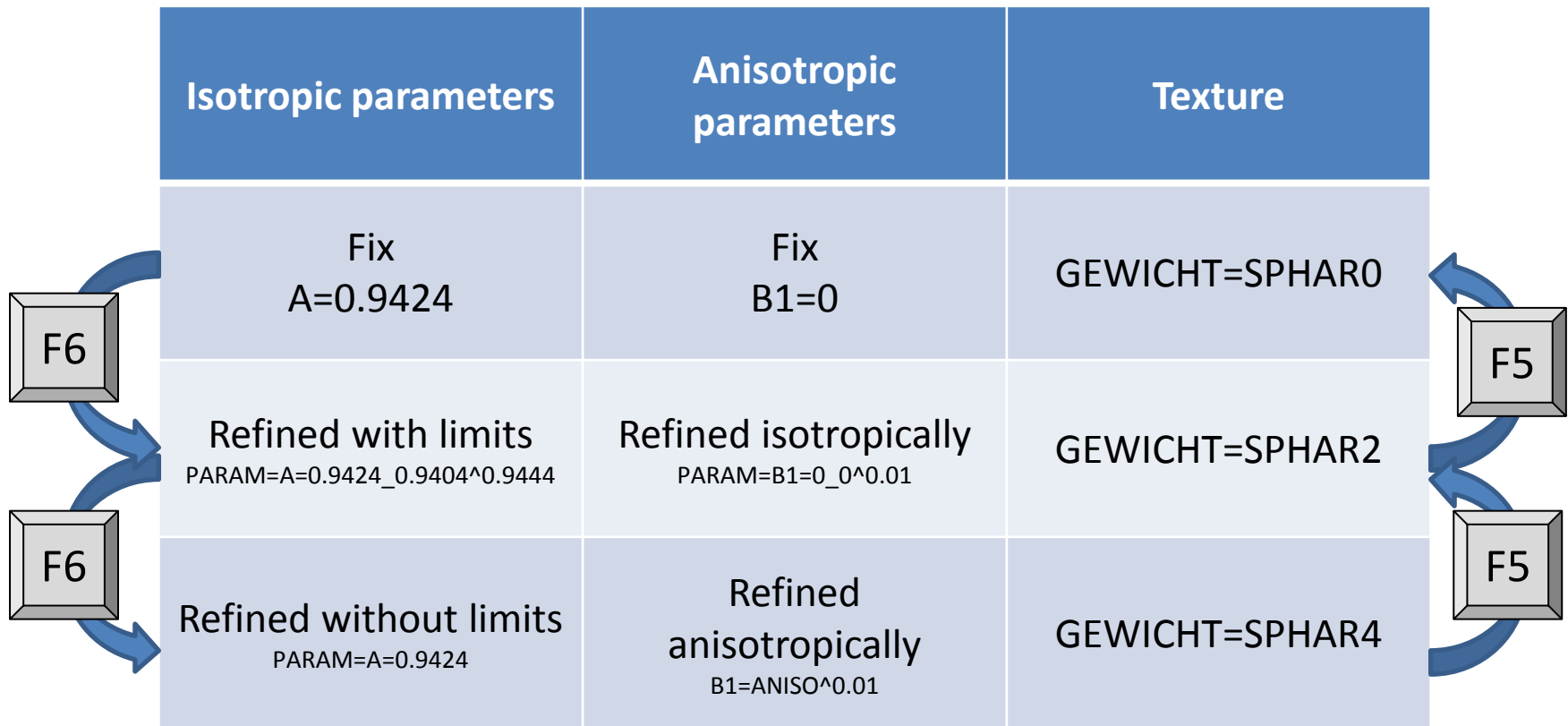
Callout Box: In «hydroxyapatite.str» right-click on «k2=0» and select «refine isotropically»

Alternatively: Place cursor on «k2=0» and press:

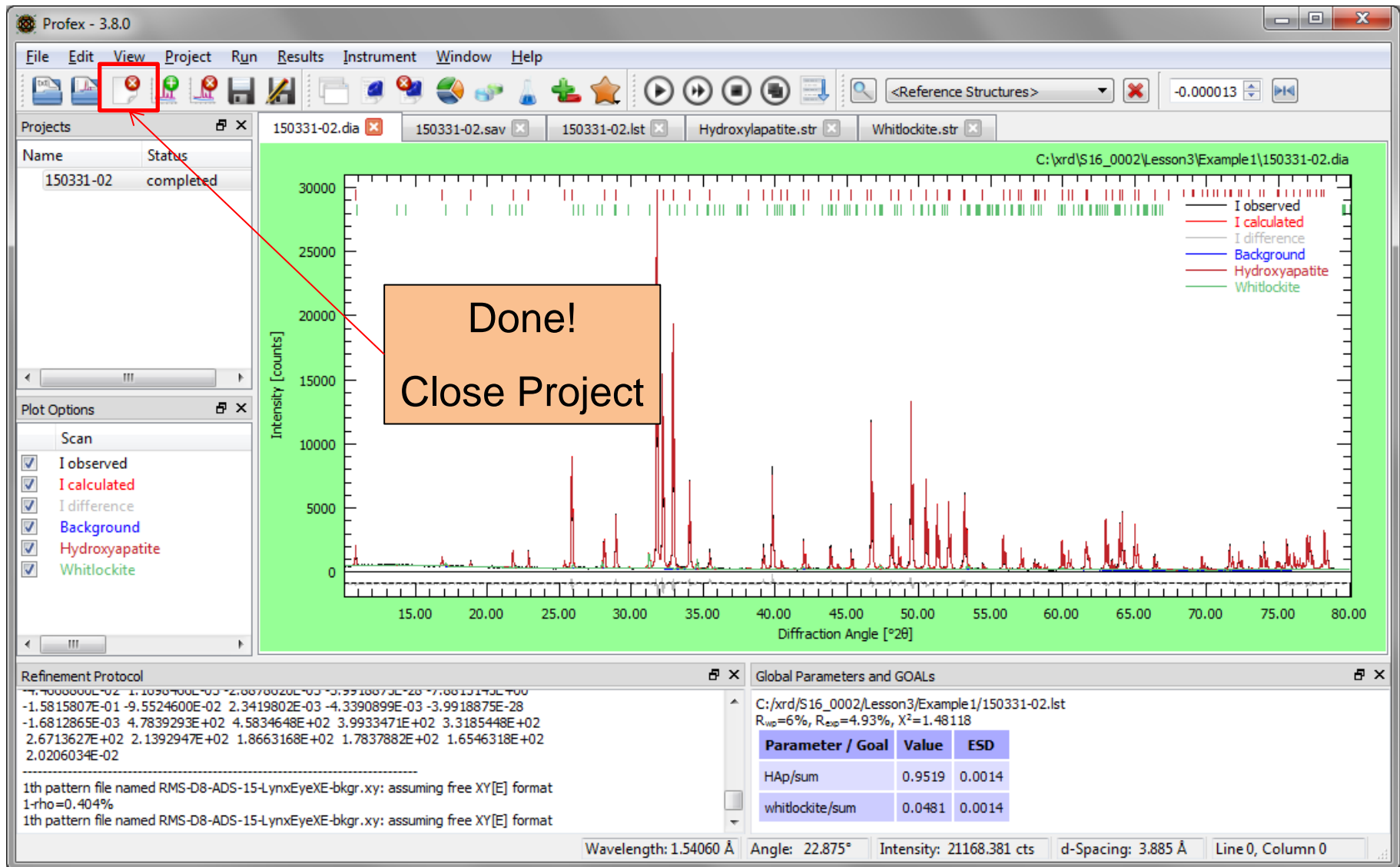
F6: fix → isotropic → anisotropic

F5: anisotropic → isotropic → fix

Toggleing Parameter Refinement States

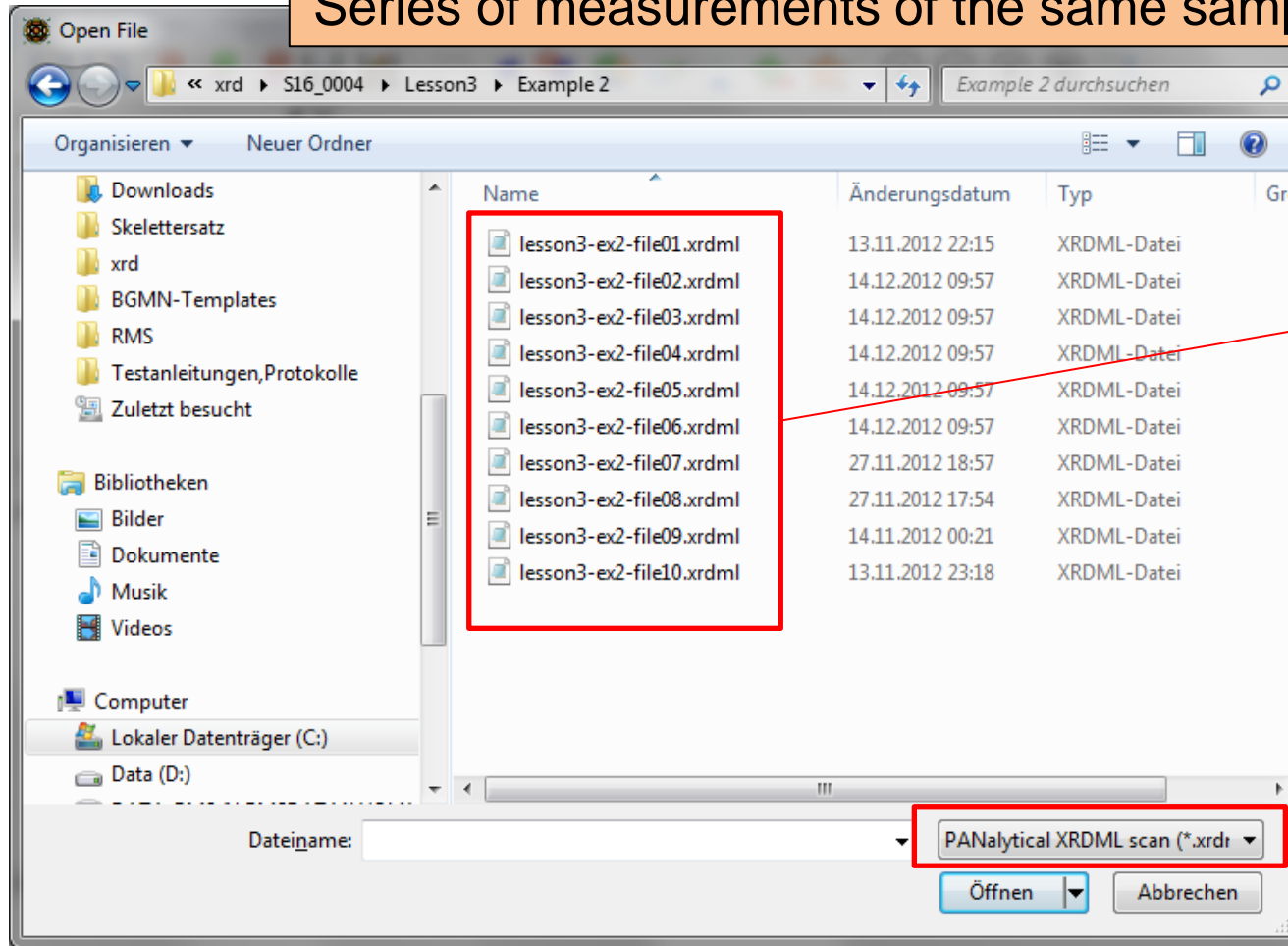


Optimized Refinement



Example 2: Batch Refinement

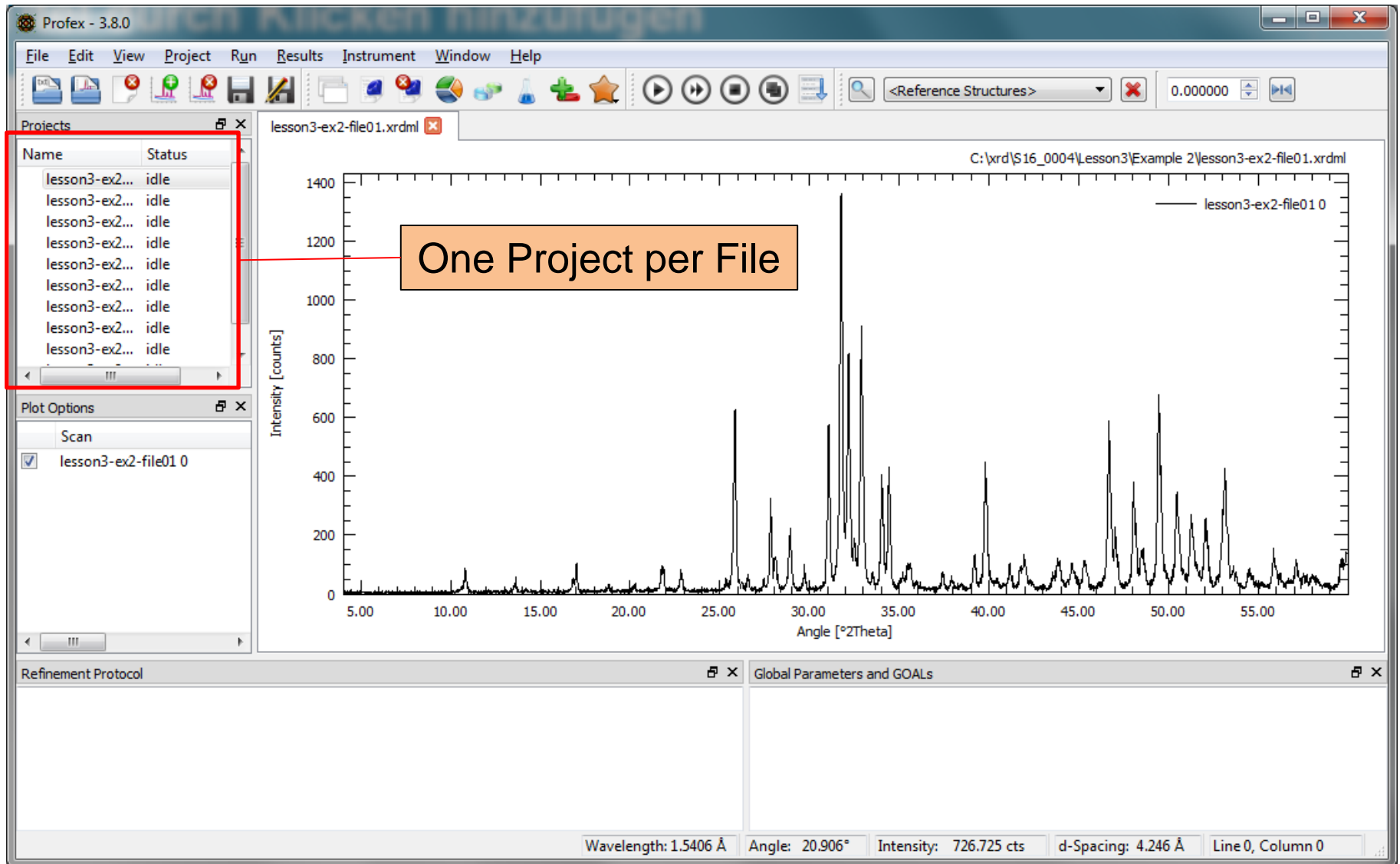
Series of measurements of the same sample



2. Select and open all files

1. Set Format

Example 2: Batch Refinement



Example 2: Batch Refinement

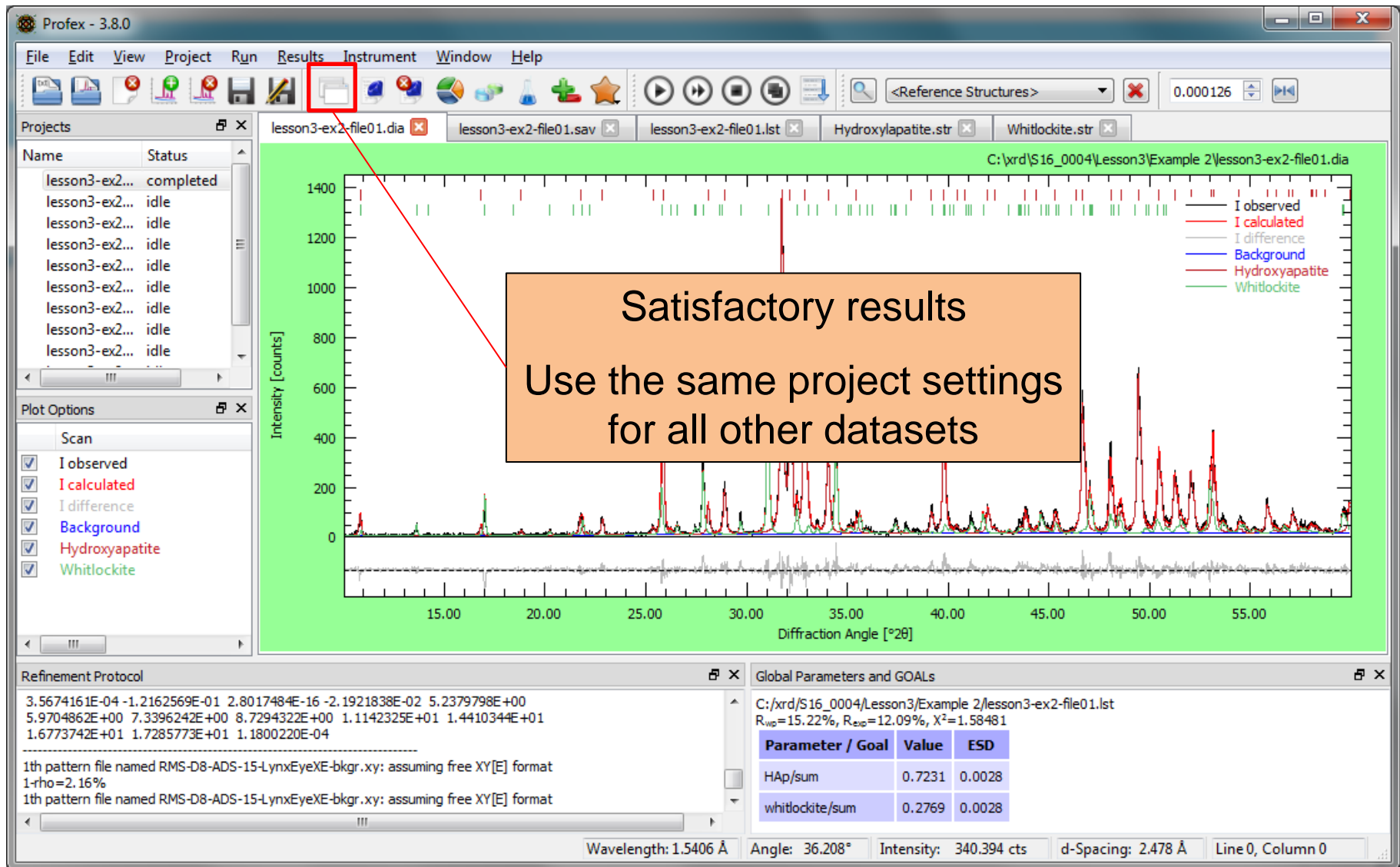
The screenshot displays the Profex 3.8.0 software interface. The main window shows a list of projects on the left, a central panel with a list of parameters and their values, and a bottom panel for refinement protocols. Two red boxes highlight the 'Add' (+) and 'Run' (play) buttons in the toolbar. Two callout boxes provide instructions: '1. Add «Hydroxyapatite» and «Whitlockite»' and '2. Run the refinement'.

1. Add «Hydroxyapatite» and «Whitlockite»

2. Run the refinement

Wavelength: 1.5406 Å Angle: 0.000° Intensity: 0.000 cts d-Spacing: 0.000 Å Line 0, Column 0

Example 2: Batch Refinement



Example 2: Batch Refinement

Profex - 3.8.0

File Edit View Project Run Results Instrument Window Help

lesson3-ex2-file02.xrdml lesson3-ex2-file02.sav*

C:\xrd\S16_0004\Lesson3\Example 2\lesson3-ex2-file02.xrdml

Intensity [counts]

Angle [°2Theta]

lesson3-ex2-file02 0

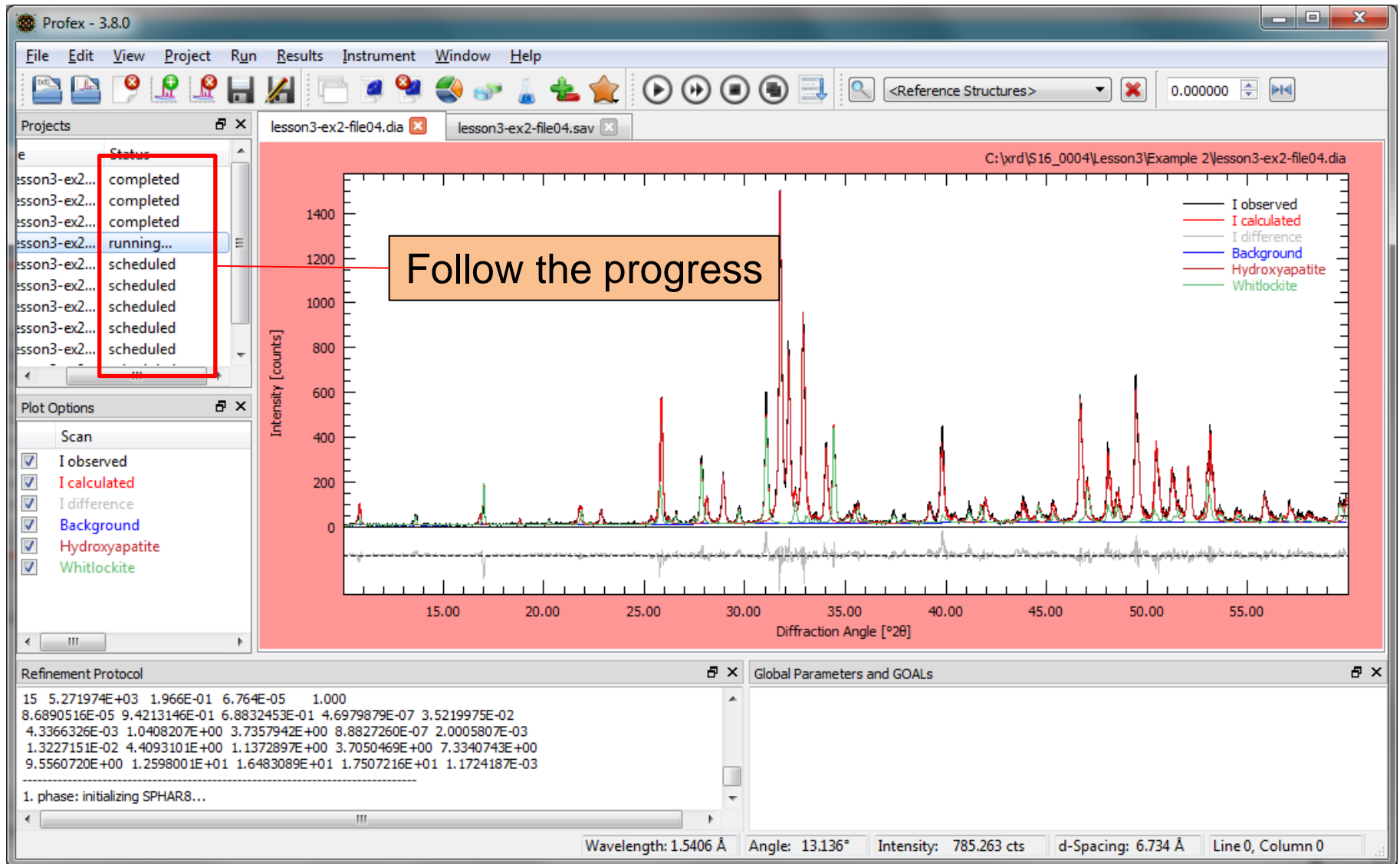
Refinement Protocol Global Parameters and GOALS

Wavelength: 1.5406 Å Angle: 21.184° Intensity: 911.444 cts d-Spacing: 4.191 Å Line 0, Column 0

Identical control file was created

«Run Batch Refinement» Will process all open projects

Example 2: Batch Refinement



Example 2: Batch Refinement

Profex - 3.8.0

File Edit View Project Run Results Instrument Window Help

Projects

Name	Status
lesson3-ex2...	completed
lesson3-ex2...	completed
lesson3-ex2...	completed
lesson3-ex2...	completed
lesson3-ex2...	completed
lesson3-ex2...	completed
lesson3-ex2...	completed
lesson3-ex2...	completed
lesson3-ex2...	completed
lesson3-ex2...	completed
lesson3-ex2...	completed

Plot Options

Scan

- I observed
- I calculated
- I difference
- Background
- Hydroxyapatite
- Whitlockite

Refinement Protocol

Global Parameters and GOALS

C:/xrd/S16_0004/Lesson3/Example 2/lesson3-ex2-file10.lst
 $R_{wp}=15\%$, $R_{exp}=12.1\%$, $X^2=1.53678$

Parameter / Goal	Value	ESD
HAp/sum	0.7213	0.0027
whitlockite/sum	0.2787	0.0027

Wavelength: 1.5406 Å Angle: 21.760° Intensity: 724.745 cts d-Spacing: 4.078 Å Line 0, Column 0

Export results of all open projects

Exported Global GOALS

The screenshot shows a Microsoft Excel spreadsheet titled 'results.csv'. The data is organized into columns: A (File), B (Sample), C (Parameter / Goal), D (Value), and E (ESD). The rows represent different test files and their associated parameters and results. A callout box highlights the 'Parameter / Goal' column with the text 'Sort by «Parameter/Goal»'.

File	Sample	Parameter / Goal	Value	ESD
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file01.lst	lesson3-ex2-file01	HAp/sum	0.7231	0.0028
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file01.lst	lesson3-ex2-file01	whitlockite/sum	0.2769	0.0028
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file01.lst	lesson3-ex2-file01	Rwp	15.22	
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file01.lst	lesson3-ex2-file01	Rexp	12.09	
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file01.lst	lesson3-ex2-file01	Chi2	1.5848	
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file02.lst	lesson3-ex2-file02	HAp/sum	0.7242	0.0027
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file02.lst	lesson3-ex2-file02	whitlockite/sum	0.2758	0.0027
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file02.lst	lesson3-ex2-file02	Rwp	14.92	
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file02.lst	lesson3-ex2-file02	Rexp	12.02	
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file02.lst	lesson3-ex2-file02	Chi2	1.5407	
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file03.lst	lesson3-ex2-file03	HAp/sum	0.725	0.0028
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file03.lst	lesson3-ex2-file03	whitlockite/sum	0.275	0.0028
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file03.lst	lesson3-ex2-file03	Rwp	15.16	
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file03.lst	lesson3-ex2-file03	Rexp	12.04	
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file03.lst	lesson3-ex2-file03	Chi2	1.5854	
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file04.lst	lesson3-ex2-file04	HAp/sum	0.7196	0.0027
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file04.lst	lesson3-ex2-file04	whitlockite/sum	0.2804	0.0027
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file04.lst	lesson3-ex2-file04	Rwp	14.8	
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file04.lst	lesson3-ex2-file04	Rexp	12.01	
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file04.lst	lesson3-ex2-file04	Chi2	1.5186	
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file05.lst	lesson3-ex2-file05	HAp/sum	0.7213	0.0027
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file05.lst	lesson3-ex2-file05	whitlockite/sum	0.2787	0.0027
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file05.lst	lesson3-ex2-file05	Rwp	14.94	
C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file05.lst	lesson3-ex2-file05	Rexp	12.05	

Exported Global GOALS

results.csv - Microsoft Excel

ZÄHLENWENN $=100 * \text{MITTELWERT}(D12:D21)$

	A	B	C	D	E	F	G	H
1	File	Sample	Parameter / Goal	Value	ESD			
2	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file01.lst	lesson3-ex2-file01	HAp/sum	0.7231	0.0028			
3	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file02.lst	lesson3-ex2-file02	HAp/sum	0.7242	0.0027			
4	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file03.lst	lesson3-ex2-file03	HAp/sum	0.725	0.0028			
5	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file04.lst	lesson3-ex2-file04	HAp/sum	0.7196	0.0027			
6	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file05.lst	lesson3-ex2-file05	HAp/sum	0.7213	0.0027			
7	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file06.lst	lesson3-ex2-file06	HAp/sum	0.722	0.0027			
8	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file07.lst	lesson3-ex2-file07	HAp/sum	0.7266	0.0027			
9	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file08.lst	lesson3-ex2-file08	HAp/sum	0.7229	0.0027			
10	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file09.lst	lesson3-ex2-file09	HAp/sum	0.7254	0.0027			
11	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file10.lst	lesson3-ex2-file10	HAp/sum	0.7213	0.0027	72.31	0.22	
12	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file01.lst	lesson3-ex2-file01	whitlockite/sum	0.2769	0.0028			
13	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file02.lst	lesson3-ex2-file02	whitlockite/sum	0.2758	0.0027			
14	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file03.lst	lesson3-ex2-file03	whitlockite/sum	0.275	0.0028			
15	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file04.lst	lesson3-ex2-file04	whitlockite/sum	0.2804	0.0027			
16	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file05.lst	lesson3-ex2-file05	whitlockite/sum	0.2787	0.0027			
17	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file06.lst	lesson3-ex2-file06	whitlockite/sum	0.278	0.0027			
18	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file07.lst	lesson3-ex2-file07	whitlockite/sum	0.2734	0.0027			
19	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file08.lst	lesson3-ex2-file08	whitlockite/sum	0.2771	0.0027			
20	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file09.lst	lesson3-ex2-file09	whitlockite/sum	0.2746	0.0027			
21	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file10.lst	lesson3-ex2-file10	whitlockite/sum	0.2787	0.0027	D12:D21	0.22	
22								
23								
24								
25								

Easy to compute mean and standard deviations

Refined Chemical Composition

Open «Window → Chemistry»

	Quantity Goal	MgO wt-%	P2O5 wt-%	CaO wt-%	Fe2O3 wt-%
Hydroxyapatite	-	0.00	43.16	56.84	0.00
Whitlockite	whitlockite/su	0.99	13.21	13.51	0.17
Total					

← Normalized to 100%

Make sure the Quantity GOALS are assigned correctly

	Quantity Goal	MgO wt-%	P2O5 wt-%	CaO wt-%	Fe2O3 wt-%
Hydroxyapatite	HAp/sum	0.00	31.13	41.00	0.00
Whitlockite	whitlockite/su	0.99	13.21	13.51	0.17
Total		0.99	44.34	54.51	0.17

← Normalized to refined phase quantity

← Total sample composition available

Create CIF files from refined structures

Profex - 3.8.0

File Edit View Project Run Results Instrument Window Help

Export Global Parameters and GOALS... Ctrl+E
Export Local Parameters and GOALS... Ctrl+Shift+E
Export Chemistry...
Export CIF files from LST file...
Export CELL files from RES file...

Projects

Name	Status
lesson3-ex2...	completed
lesson3-ex2...	completed
lesson3-ex2...	completed
lesson3-ex2...	completed
lesson3-ex2...	completed
lesson3-ex2...	completed
lesson3-ex2...	completed
lesson3-ex2...	completed
lesson3-ex2...	completed
lesson3-ex2...	completed

Plot Options

Scan

- I observed
- I calculated
- I difference
- Background
- Hydroxyapatite
- Whitlockite

Intensity [counts]

Diffraction Angle [°2θ]

Export CIF files

Refinement Protocol

1th pattern file named RMS-D8-ADS-15-LynxEyeXE-bkgr.xy: assuming free XY[E] format
1-rho=2.11%
1th pattern file named RMS-D8-ADS-15-LynxEyeXE-bkgr.xy: assuming free XY[E] format
Exported CIF files:
C:/xrd/S16_0004/Lesson3/Example 2/lesson3-ex2-file10-Hydroxyapatite.cif
C:/xrd/S16_0004/Lesson3/Example 2/lesson3-ex2-file10-Whitlockite.cif

Global Parameters and GOALS

C:/xrd/S16_0004/Lesson3/Example 2/lesson3-ex2-file10.lst
R_{wp}=15%, R_{exp}=12.1%, X²=1.53678

Parameter / Goal	Value	ESD
HAp/sum	0.7213	0.0027
whitlockite/sum	0.2787	0.0027

Wavelength: 1.5406 Å Angle: 22.793° Intensity: 1147.845 cts d-Spacing: 3.895 Å Line 0, Column 0

Drawing Structures

lesson3-ex2-file10-Hydroxyapatite.cif

File Edit View Objects Utilities Help

a b c a* b* c* Step (°): 10.0 Step (px): 50 Step (%): 50

Tools Style Objects

Structural models

- Show models
- Show dot surface

Style

- Ball-and-stick
- Space-filling
- Polyhedral
- Wireframe
- Stick

Volumetric data

- Show sections
- Show isosurfaces
- Surface coloring

Style

- Smooth shading
- Wireframe
- Dot surface

Crystal shapes

- Show shapes

Style

- Unicolor
- Custom color
- Wireframe

Properties... Boundary... Orientation...

Number of polygons and unique vertices on isosurface = 0 (0)
72 atoms, 0 bonds, 0 polyhedra; CPU time = 0 ms

76 atoms, 24 bonds, 6 polyhedra; CPU time = 1 ms

Output Comment

Exporting Diffraction Patterns

The screenshot shows the Profex 3.8.0 interface. The main plot area displays Intensity [counts] on the y-axis (0 to 1400) and Diffraction Angle [°2θ] on the x-axis (15.00 to 55.00). The plot includes observed data (black), calculated data (red), difference (grey), background (blue), Hydroxyapatite (red), and Whitlockite (green). A text box with two instructions is overlaid on the plot:

1. Display the Plot Area
2. Select «Save As...»

The interface also shows a Projects list on the left, Plot Options, and a Refinement Protocol section at the bottom. The Refinement Protocol section contains the following text:

3.5674161E-04 -1.2162569E-01 2.8017484E-16 -2.1921838E-02 5.2379798E+00
5.9704862E+00 7.3396242E+00 8.7294322E+00 1.1142325E+01 1.4410344E+01
1.6773742E+01 1.7285773E+01 1.1800220E-04

1th pattern file named RMS-D8-ADS-15-LynxEyeXE-bkgr.xy: assuming free XY[E] format
1-rho=2.16%

1th pattern file named RMS-D8-ADS-15-LynxEyeXE-bkgr.xy: assuming free XY[E] format

The Global Parameters and GOALS section shows the following data:

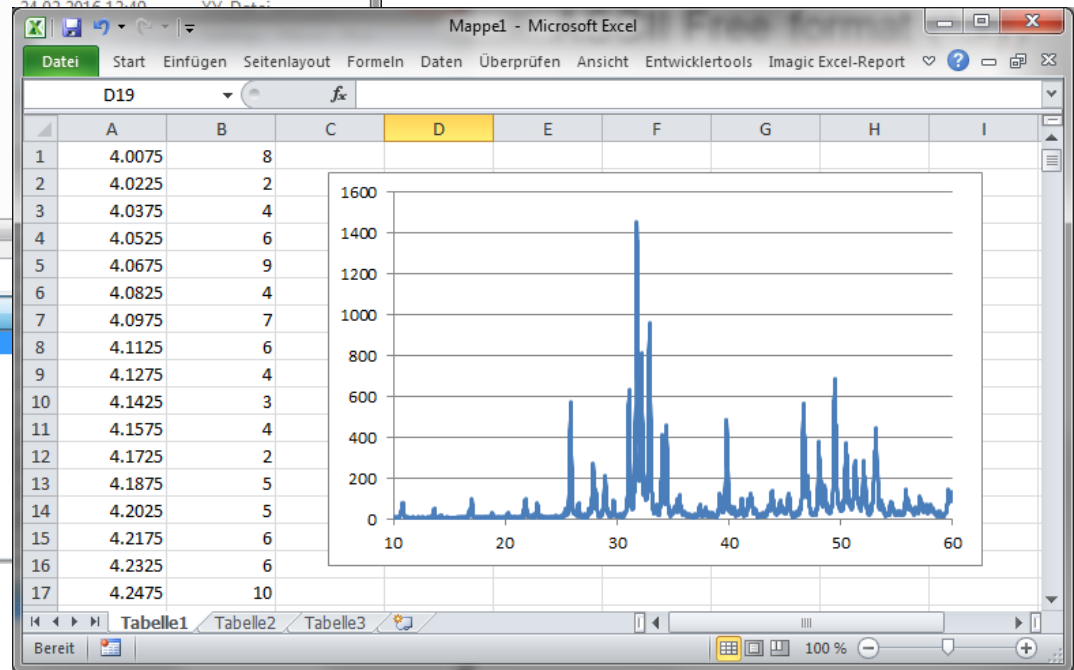
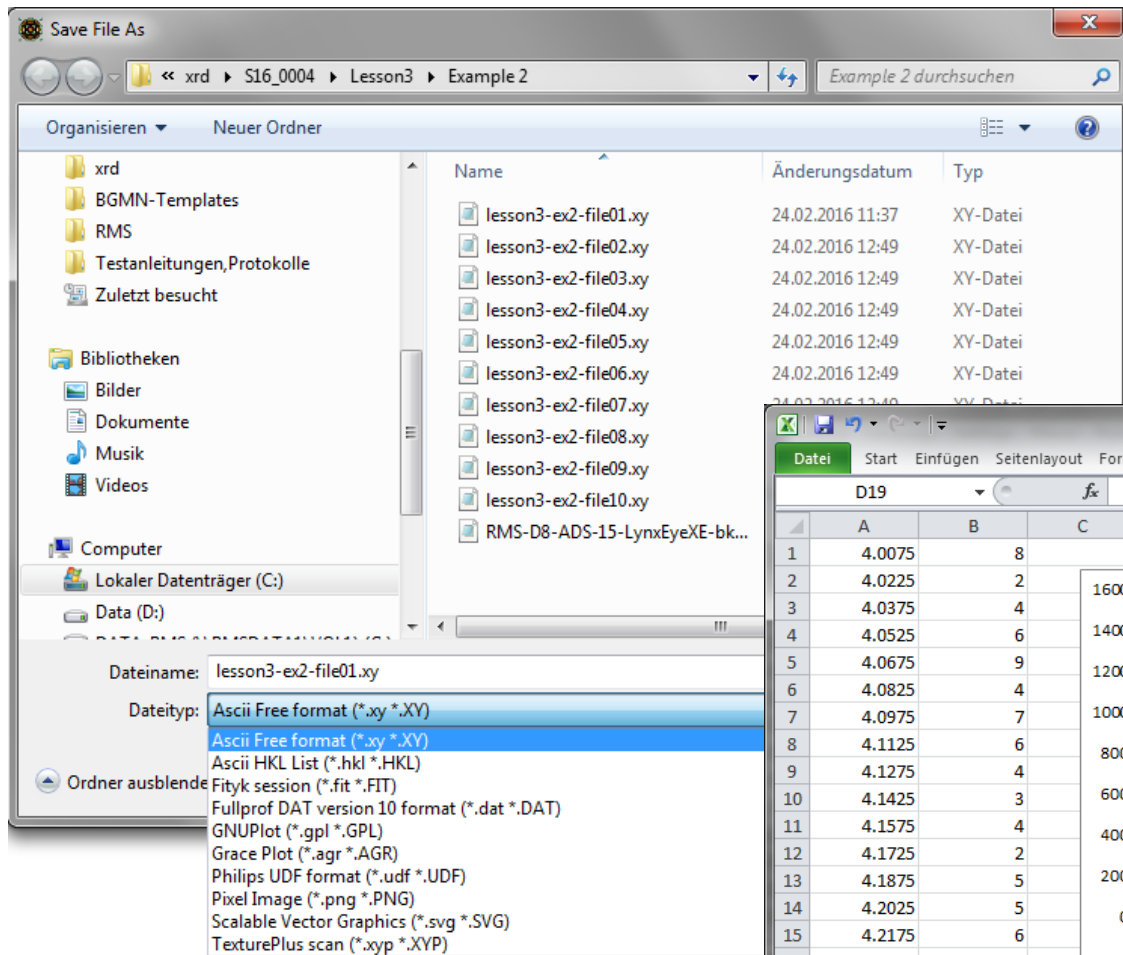
Parameter / Goal	Value	ESD
HAp/sum	0.7231	0.0028
whitlockite/sum	0.2769	0.0028

At the bottom of the interface, the following parameters are displayed: Wavelength: 1.5406 Å, Angle: 27.184°, Intensity: 976.182 cts, d-Spacing: 3.276 Å, Line 0, Column 0.

Diffraction Data Formats

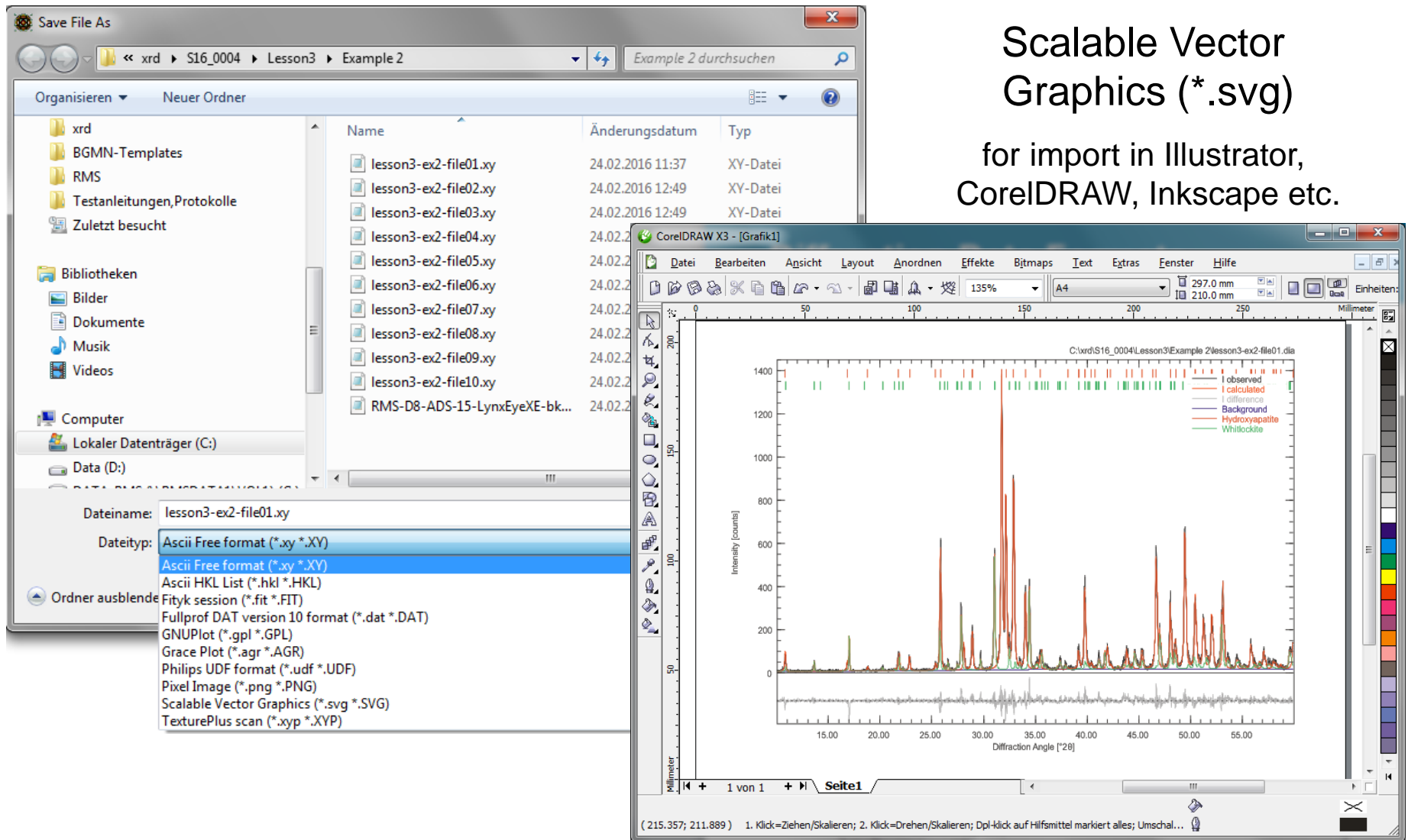
ASCII Free format (*.xy)

for import in
Excel, Origin, etc.

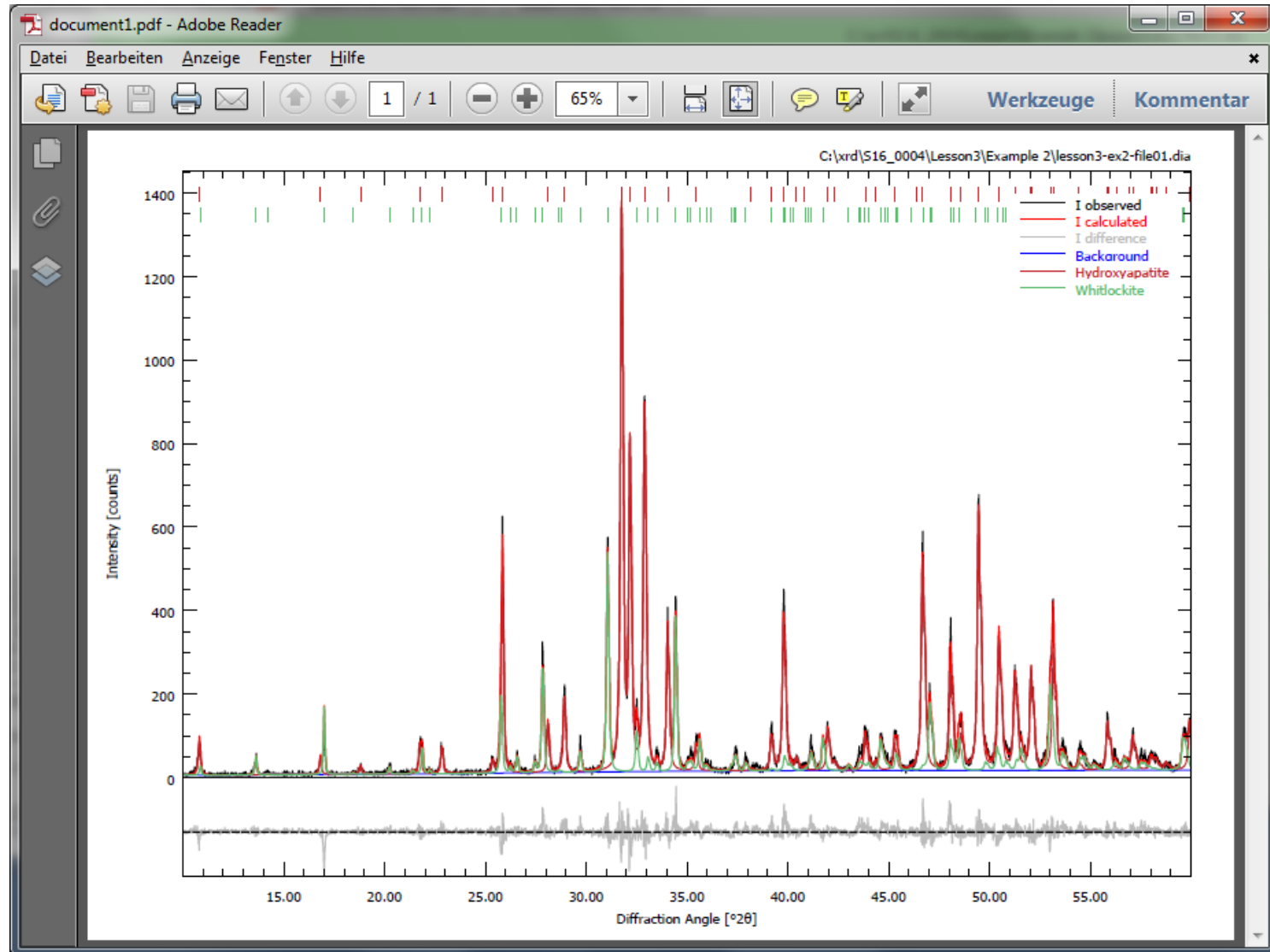


Diffraction Data Formats

Scalable Vector Graphics (*.svg)
for import in Illustrator,
CoreIDRAW, Inkscape etc.



Diffraction Data Formats



➤ More «Behind the Scenes» information in «Lesson 8: Crystal Structures»



PROFEX

OPEN SOURCE XRD AND RIETVELD REFINEMENT

[Home](#) [What's New](#) [Download](#) [Lecture Handouts](#) [Tutorials](#) [Useful Links](#) [Contact](#)

Tutorials

Instrument Configuration Files

This tutorial guides through the process of creating an instrument configuration file. [Continue...](#)

First Steps: Basic Refinement

This tutorial describes a basic refinement of a 3-phase dataset, as it is usually performed to identify and quantify the phase content. A raw data file is provided for download. [Continue...](#)

Sub-phases

This tutorial demonstrates how to use BGMN's concept of sub-phases to refine bimodal distributions of crystallite sizes due to overmilling. It also couples crystallite sizes and micro-strain of secondary phases to improve the stability and reliability of the refinement. [Continue...](#)