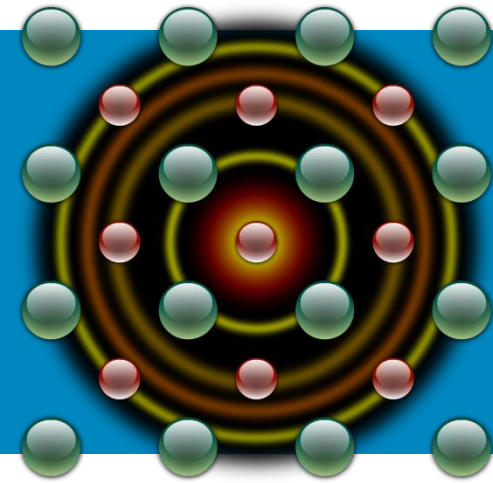


Lesson 3

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 -10.10 (64bit)

Rietveld Backends: BGMN, Fullprof.2k

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

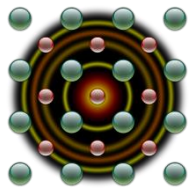
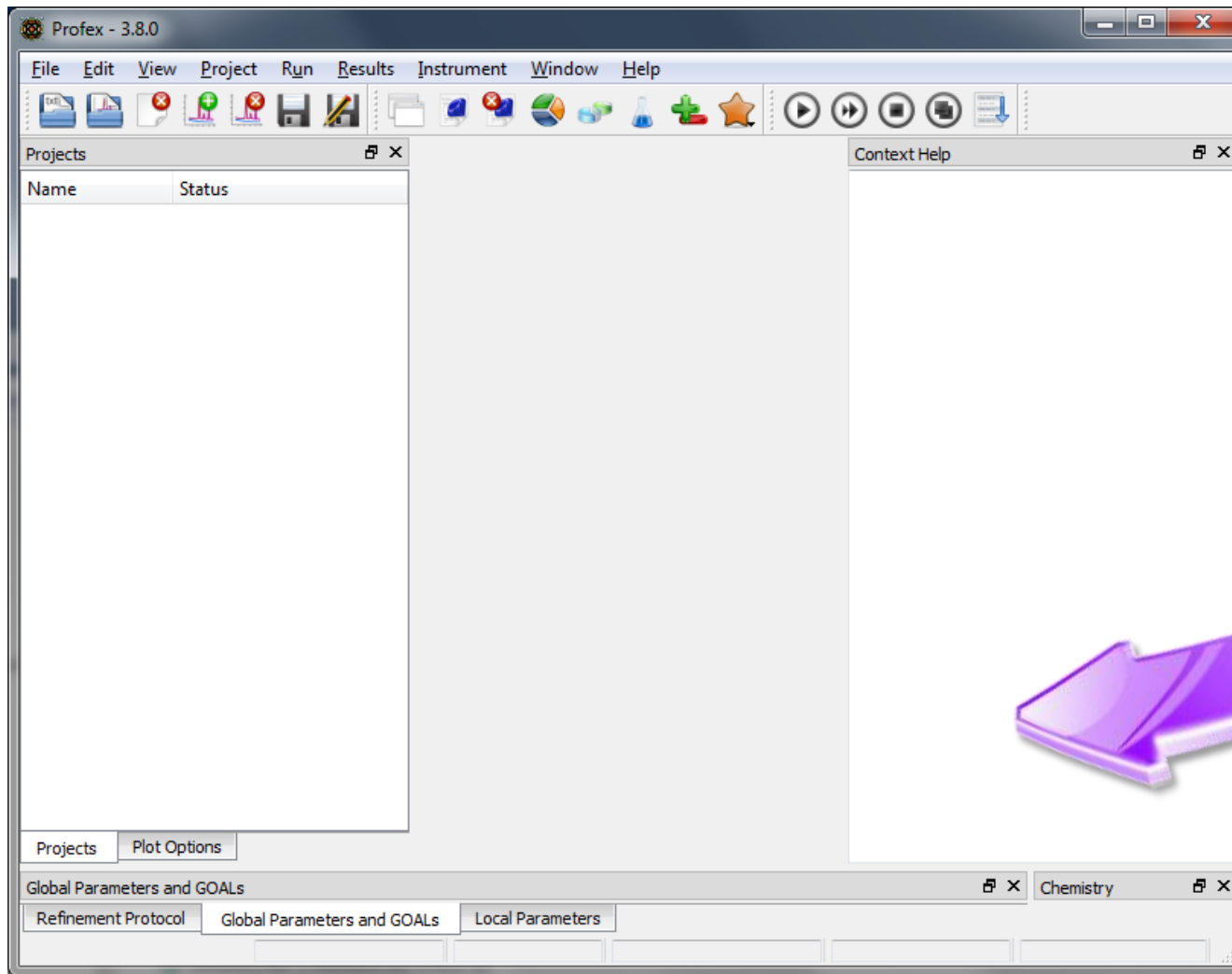
Current stable version: 3.8.0

History

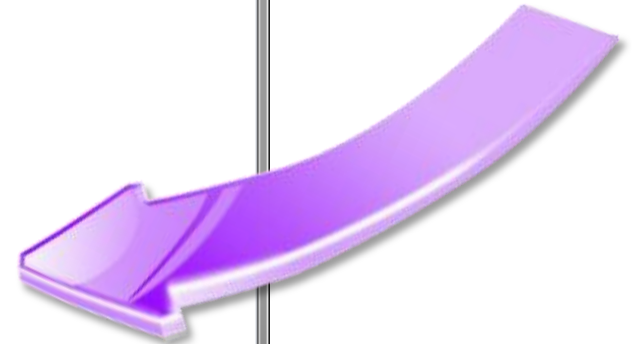
- 2003: Start of development as an alternative GUI for Fullprof.2k
For personal use only (my PhD)
Linux only
- 2006: Major rewrite
Support for Windows
- 2012: Support for BGMN Rietveld Backend added
- 2014: Support for Mac OS X



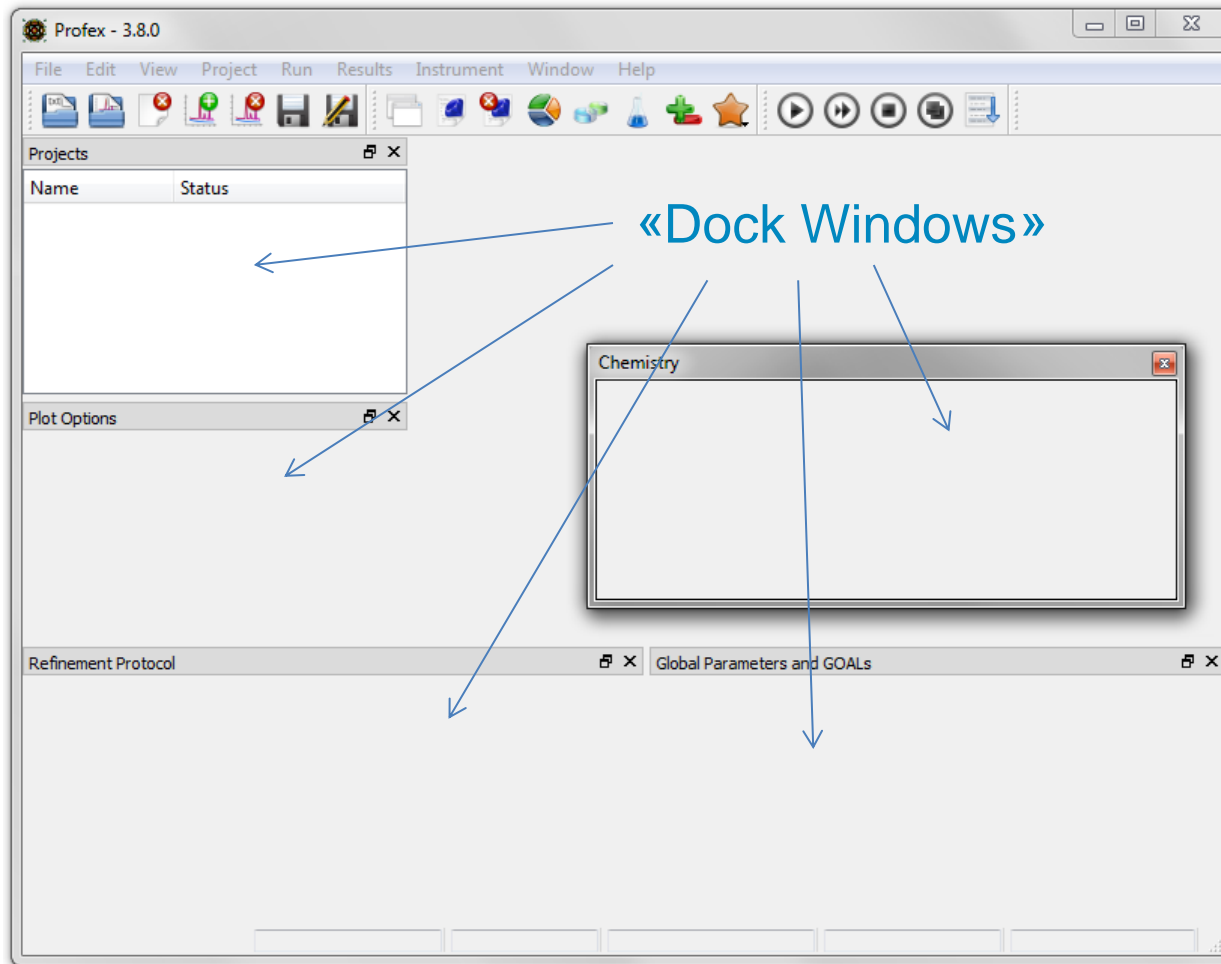
First Use



Profex



First Use



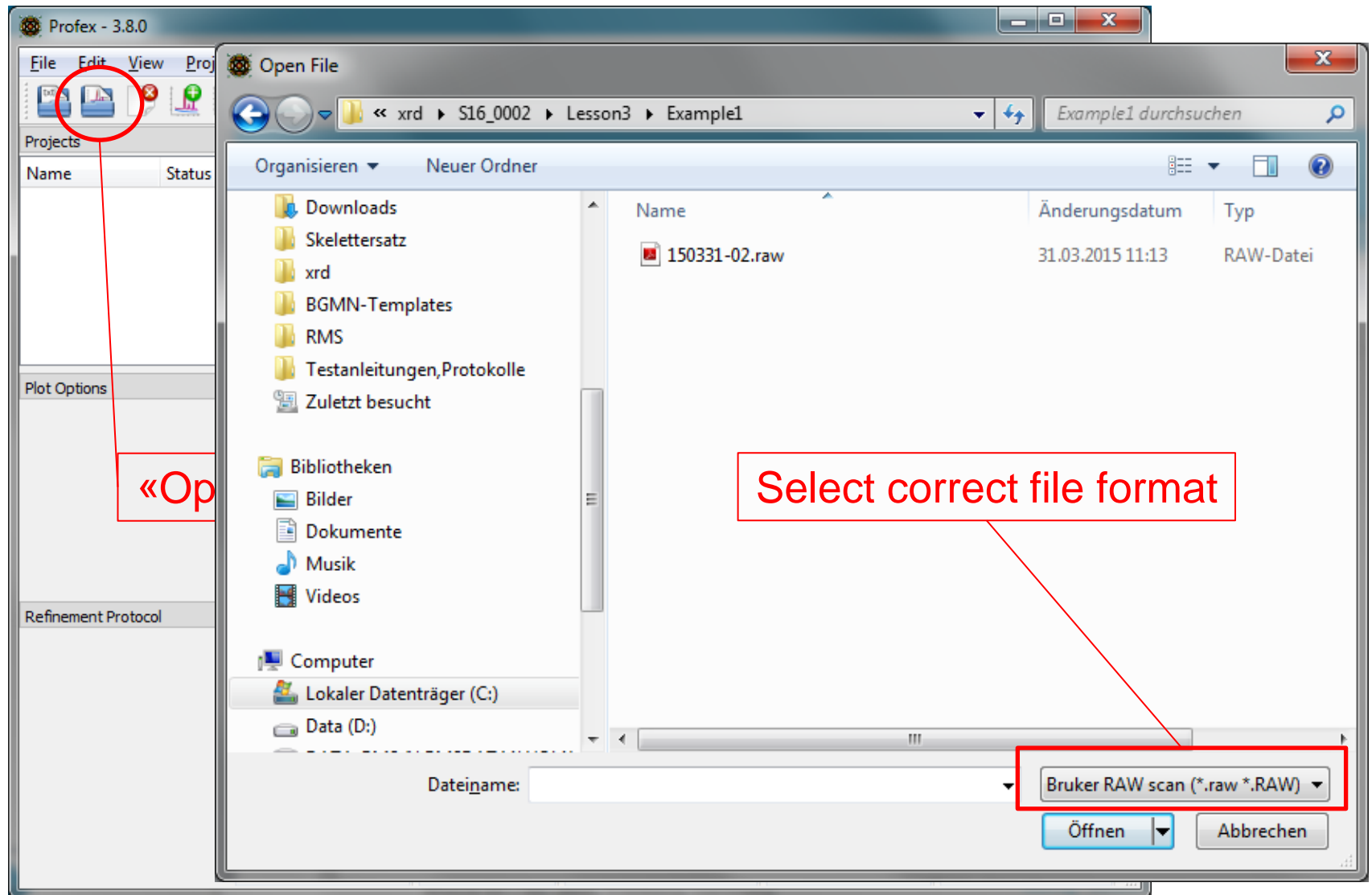
Can be re-arranged
(drag & drop)

Stacked

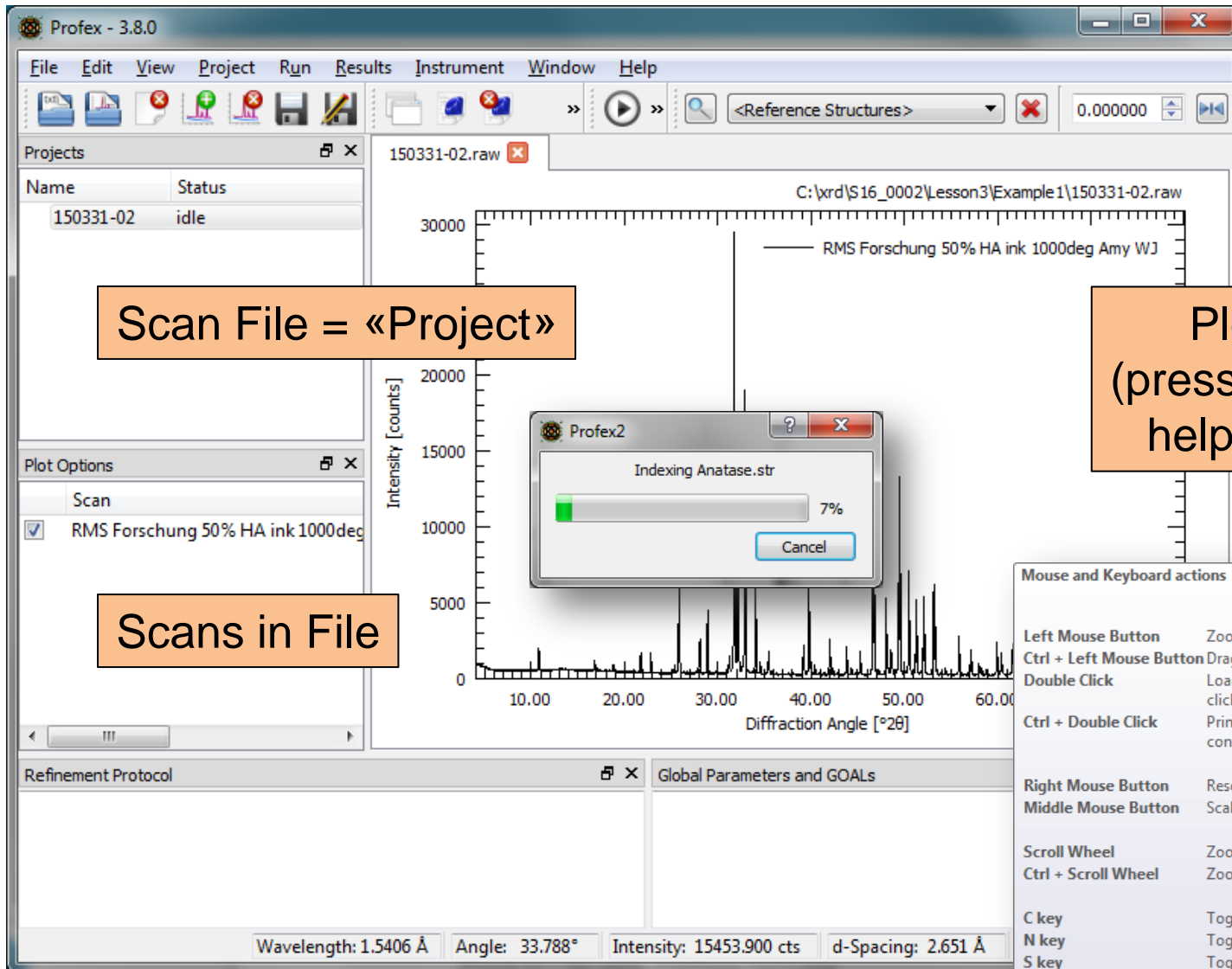
Floating

Closed
(opened from
«Window» menu)

Load Scan File



First Use: Example 1



Scan File = «Project»

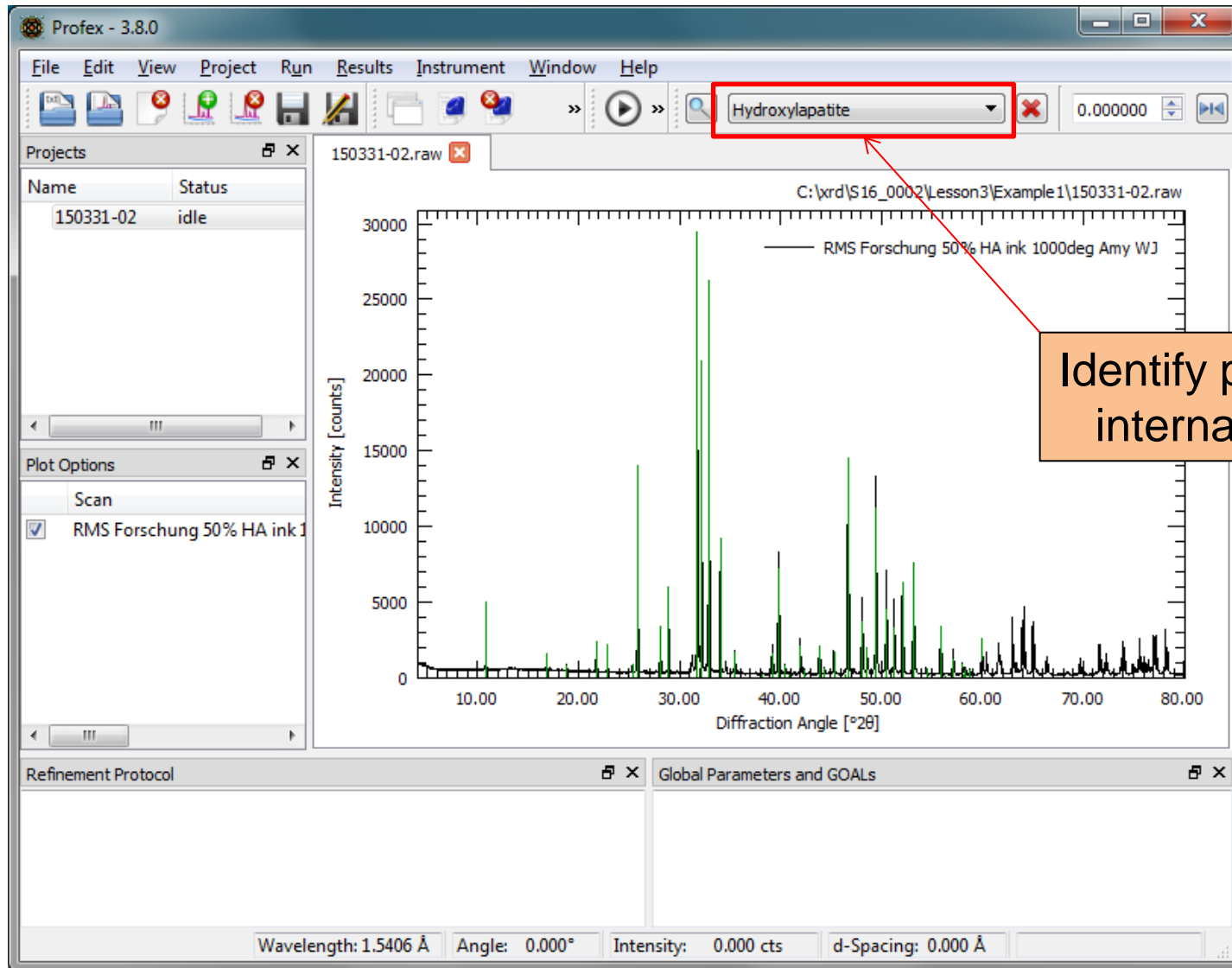
Scans in File

Plot area
(press «shift» for help window)

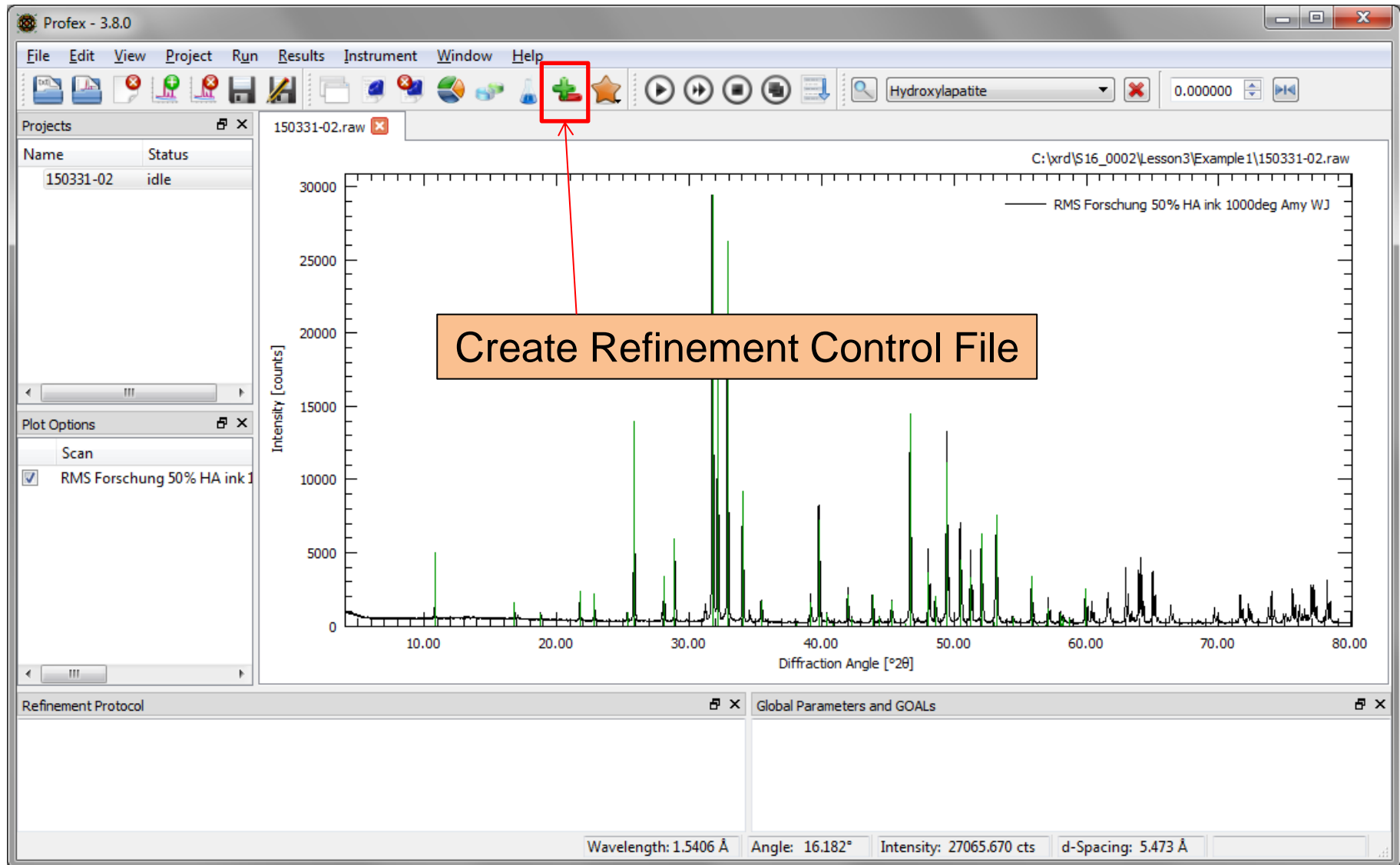
Mouse and Keyboard actions

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

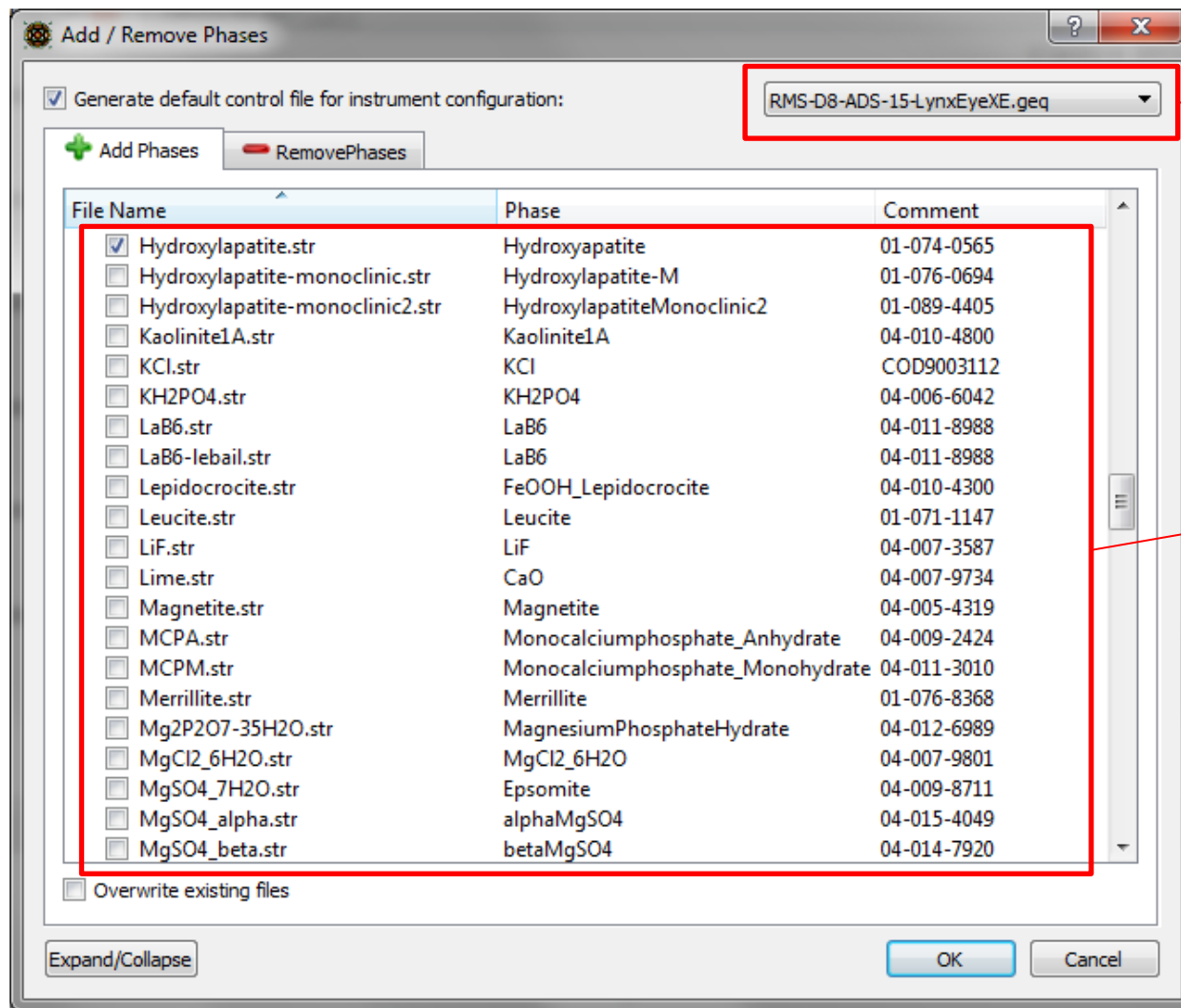
First Use: Example 1



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 shows 'RMS Forschung 50% HA ink' selected. 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/su
```

A red box highlights the '150331-02.sav*' file in the 'Projects' tab. A callout box points to this file with 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.

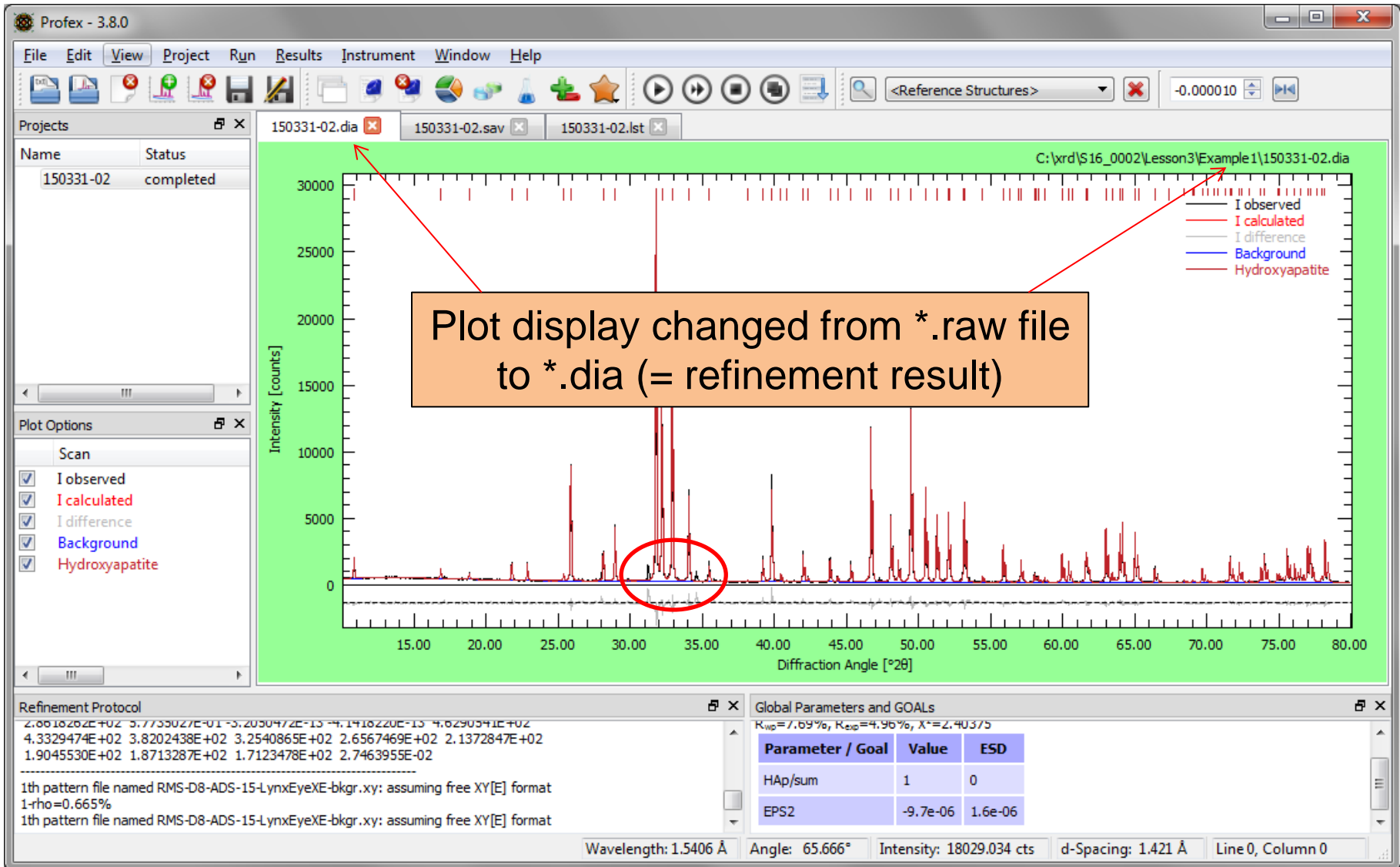
First Use: Example 1

The screenshot displays the Profex 3.8.0 software interface. The main window shows a refinement protocol for 'RMS Forschung 50% HA ink 1000deg Amy WJ'. The protocol includes parameters such as WMIN=10, WMAX=60, and STRUC[1]=Hydroxylapatite.str. A red box highlights the play button icon in the toolbar, with a callout box containing the text 'Run the refinement'. The interface also shows a 'Projects' panel on the left, a 'Plot Options' panel, and a 'Refinement Protocol' panel at the bottom. The status bar at the bottom indicates Wavelength: 1.5406 Å, Angle: 0.000°, Intensity: 0.000 cts, d-Spacing: 0.000 Å, and Line 0, Column 0.

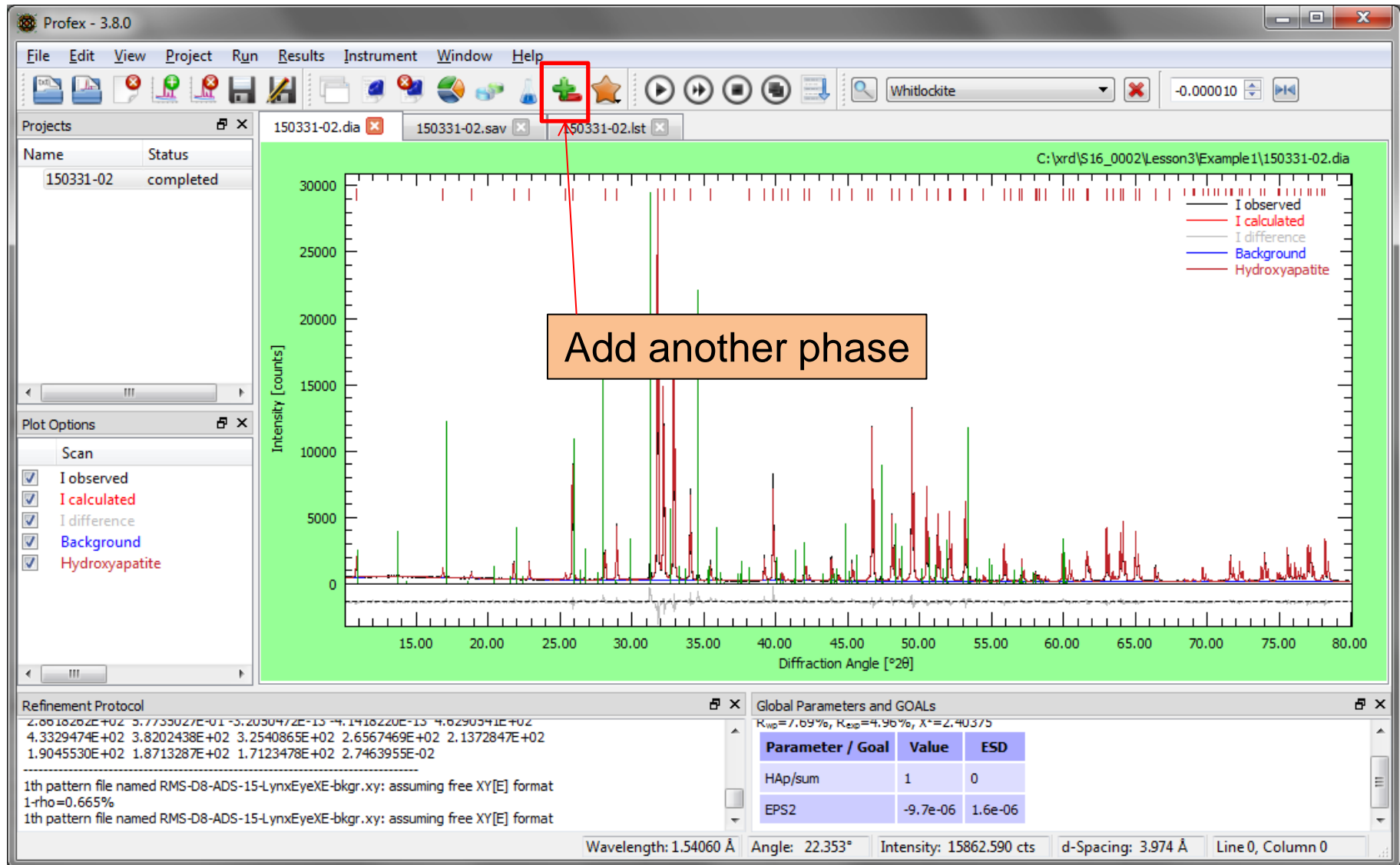
```
% SampleID: RMS Forschung 50% HA ink 1000deg Amy WJ
% Theoretical instrumental function
VERZERR=RMS-D8-ADS-15-LynxEyeXE.geq
% Wavelength
LAMBDA=CU
% Phases
STRUC[1]=Hydroxylapatite.str
% Measured background
UNT=RMS-D8-ADS-15-LynxEyeXE-bkgr.xy
% Measured data
VAL[1]=150331-02.xy
% Minimum Angle (2theta)
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/su
```

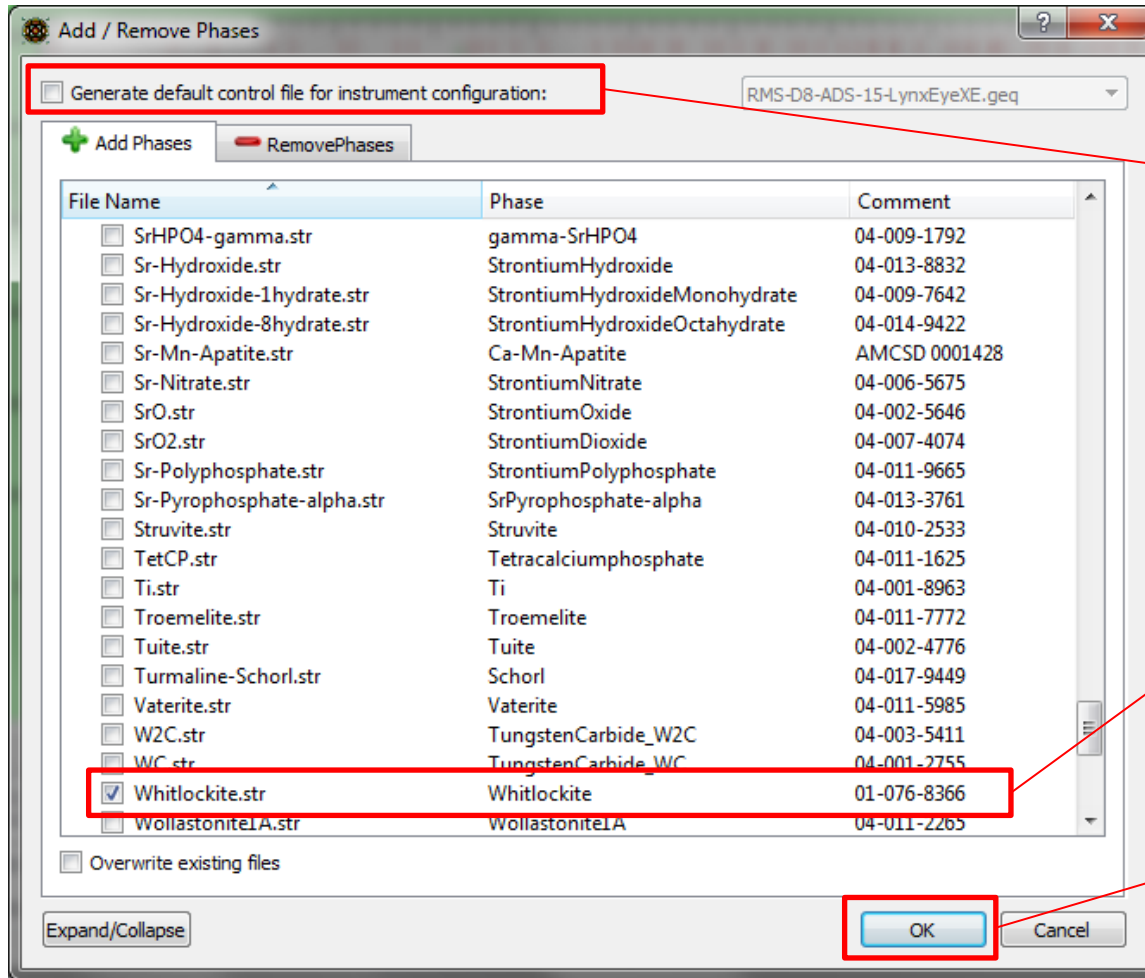
First Use: Example 1



First Use: Example 1



First Use: Example 1

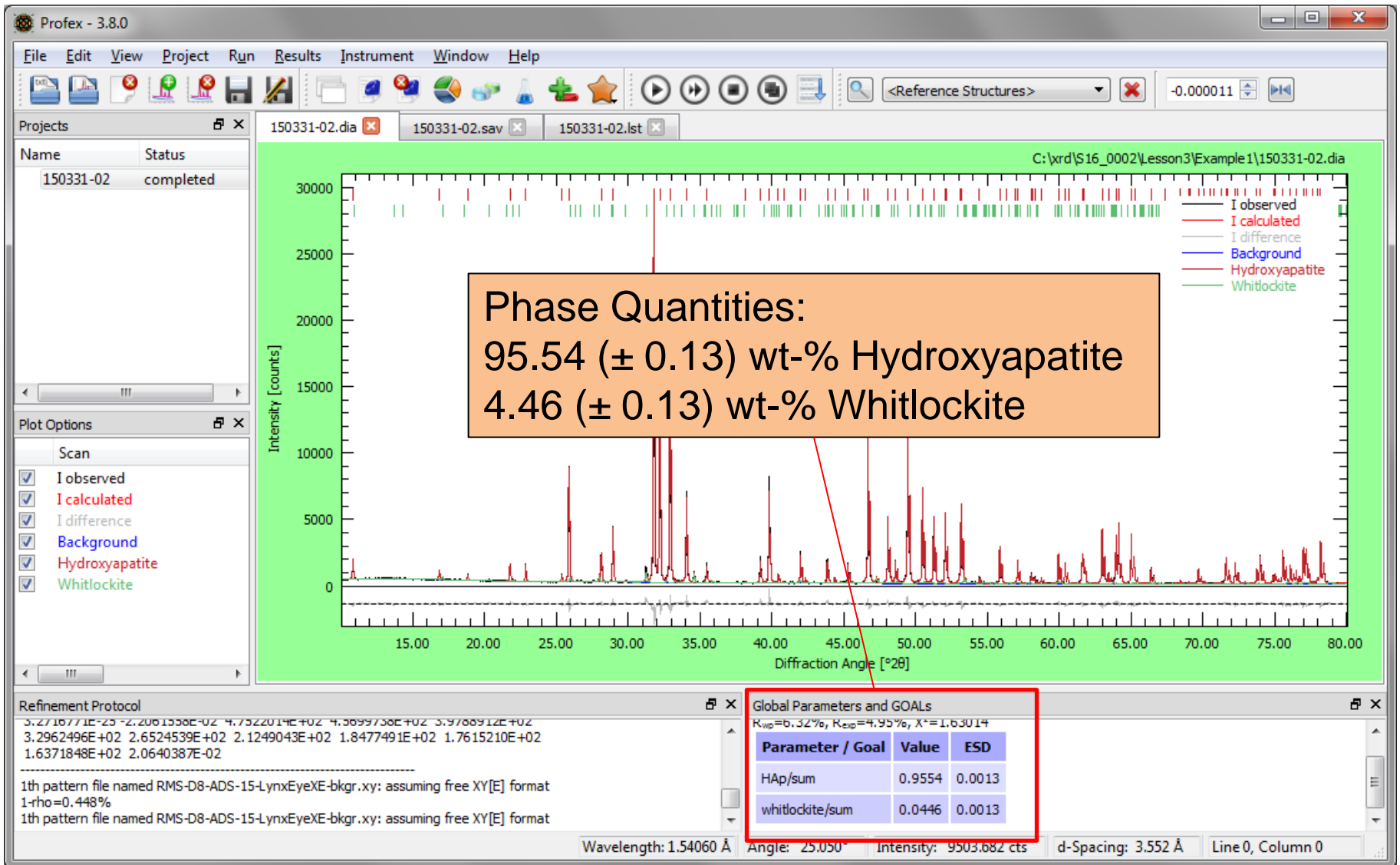


Control file already exists, **don't** generate a new default file

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

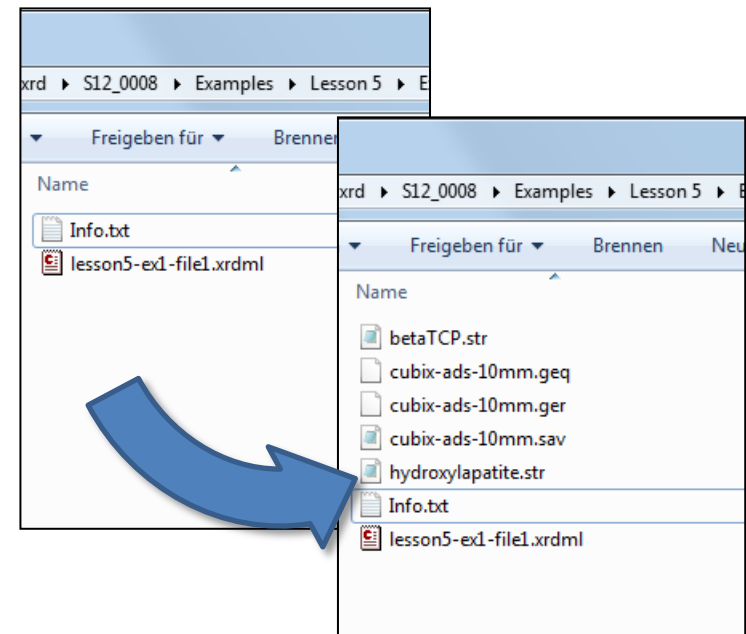
Wavelength: 1.54060 Å Angle: 0.000° Intensity: 0.000 cts d-Spacing: 0.000 Å Line 0, Column 0

*.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

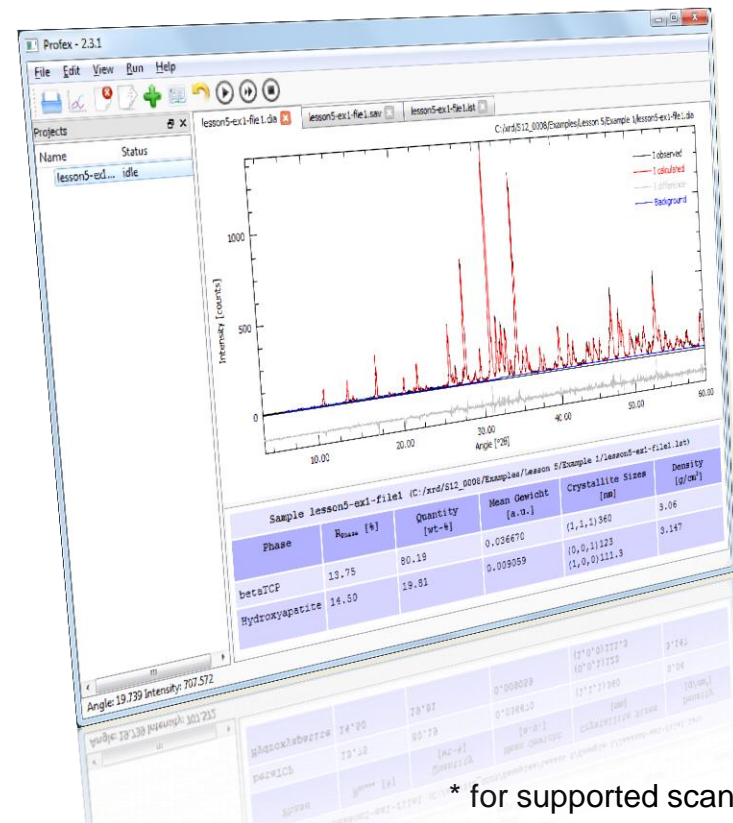
Features of Profex (III)

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
- Restrictions in terms of custom calculations
(Refinement should work, but summary table may be wrong)



Optimizing the Refinement

The screenshot shows the Profex 3.8.0 interface. The main window displays a list of files and a context menu. The context menu is open over the line «STRUC[1]=Hydroxyapatite.str». The menu options 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 FCFOOT file, and Add PDBOUT file. A red arrow points from the text box to the 'Open file' option.

**Right-click on line
«STRUC[1]=Hydroxyapatite.str»
And select
«Open File»**

The main window content includes 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
```

The Refinement Protocol window shows the following data:

```
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 window shows the following table:

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 software interface. The main window displays the refinement protocol for Hydroxylapatite. The 'Projects' panel on the left shows a project named '150331-02' with a status of 'completed'. The 'Plot Options' panel shows various options checked, including 'I observed', 'I calculated', 'I difference', 'Background', 'Hydroxyapatite', and 'Whitlockite'. The 'Refinement Protocol' panel shows the following text:

```
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_0.6810^0.6948 //
RP=4 k1=0 k2=0 B1=ANISO^0.05 GEWICHT=SPHAR4 //
GOAL=GrainSize(0,0,1) //
GOAL=GrainSize(1,0,0) //
GOAL:HAp=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1)
E=CA Wyckoff=f x=0.3333 y=0.6667 z=0.0015 TDS=0.00664290
E=CA Wyckoff=h x=0.2468 y=0.9934 z=0.2500 TDS=0.00567436
E=P Wyckoff=h x=0.3987 y=0.3685 z=0.2500 TDS=0.00477426
E=O Wyckoff=h x=0.3284 y=0.4848 z=0.2500 TDS=0.00953535
E=O Wyckoff=h x=0.5873 y=0.4651 z=0.2500 TDS=0.01014069
E=O Wyckoff=i x=0.3437 y=0.2579 z=0.0702 TDS=0.01499127
E=O(0.5000) Wyckoff=e x=0.0000 y=0.0000 z=0.1950 TDS=0.00000000
E=H(0.5000) Wyckoff=e x=0.0000 y=0.0000 z=0.0608 TDS=0.02947459
```

The 'Global Parameters and GOALS' panel shows the following table:

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

At the bottom of the interface, the following parameters are displayed: Wavelength: 1.54060 Å, Angle: 0.000°, Intensity: 0.000 cts, d-Spacing: 0.000 Å, Line 0, Column 0.

Two callout boxes provide instructions:

- A box pointing to the 'Hydroxylapatite.str' and 'Whitlockite.str' tabs in the top toolbar says: "Opens both structure files".
- A box pointing to the 'Open all Project Structure Files' icon in the top toolbar says: "Alternatively click «Open all Project Structure Files»".

Optimizing the Refinement

Profex - 3.8.0

File Edit View Project Run Results Instrument Window Help

Projects

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

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

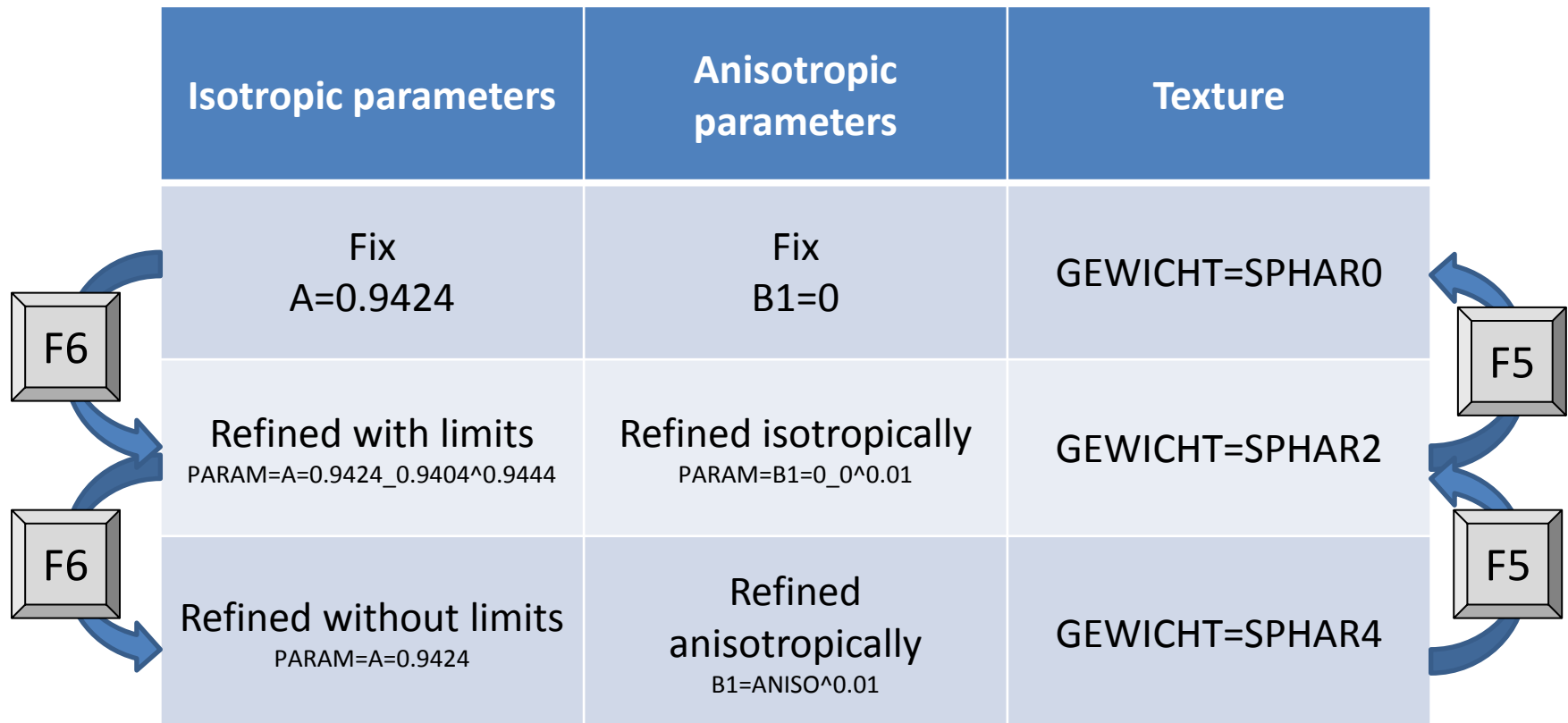
In «hydroxyapatite.str»
right-click on
«k2=0»
and select
«refine isotropically»

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

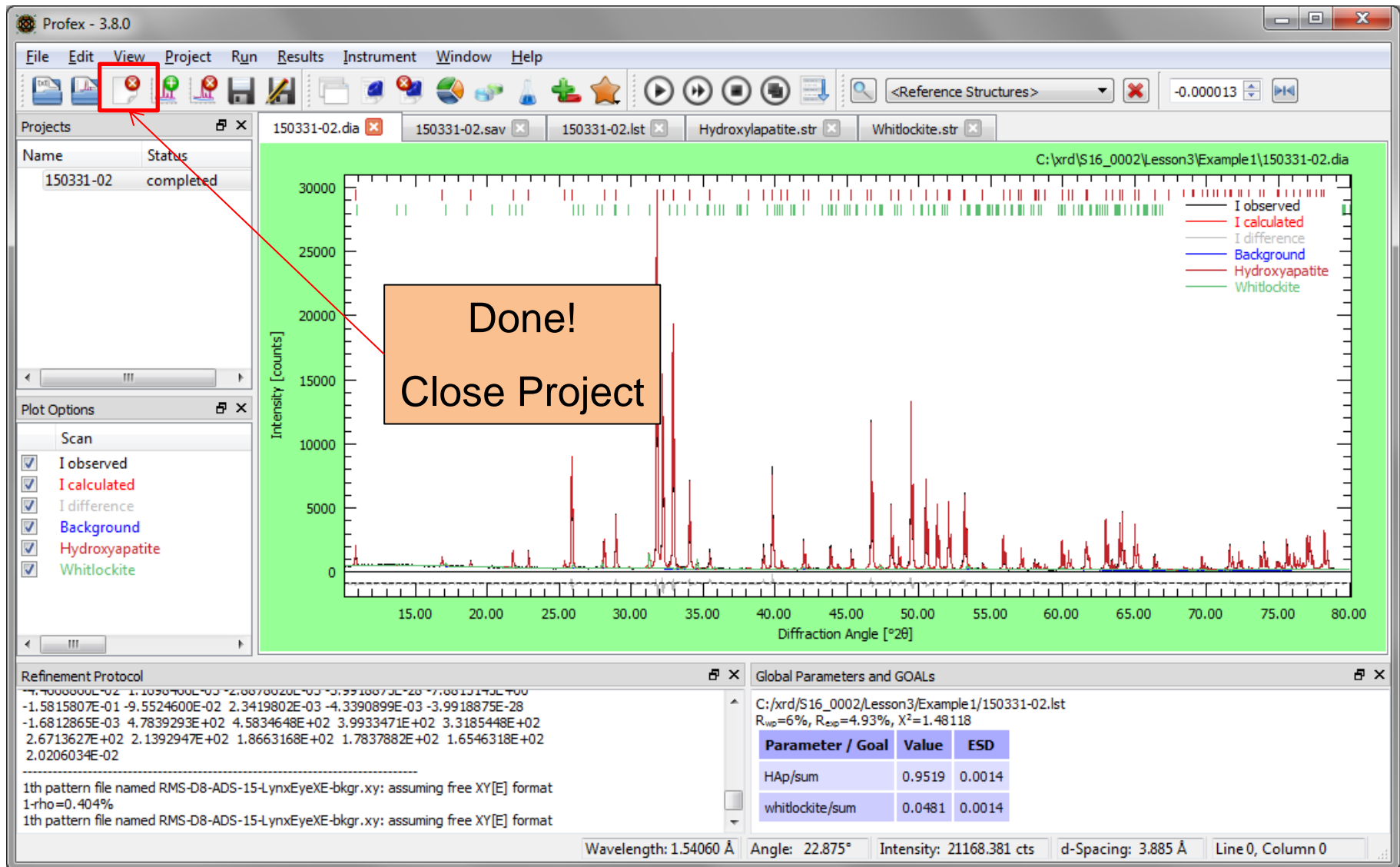
F6: fix → isotropic → anisotropic

F5: anisotropic → isotropic → fix

Toggleing Parameter Refinement States

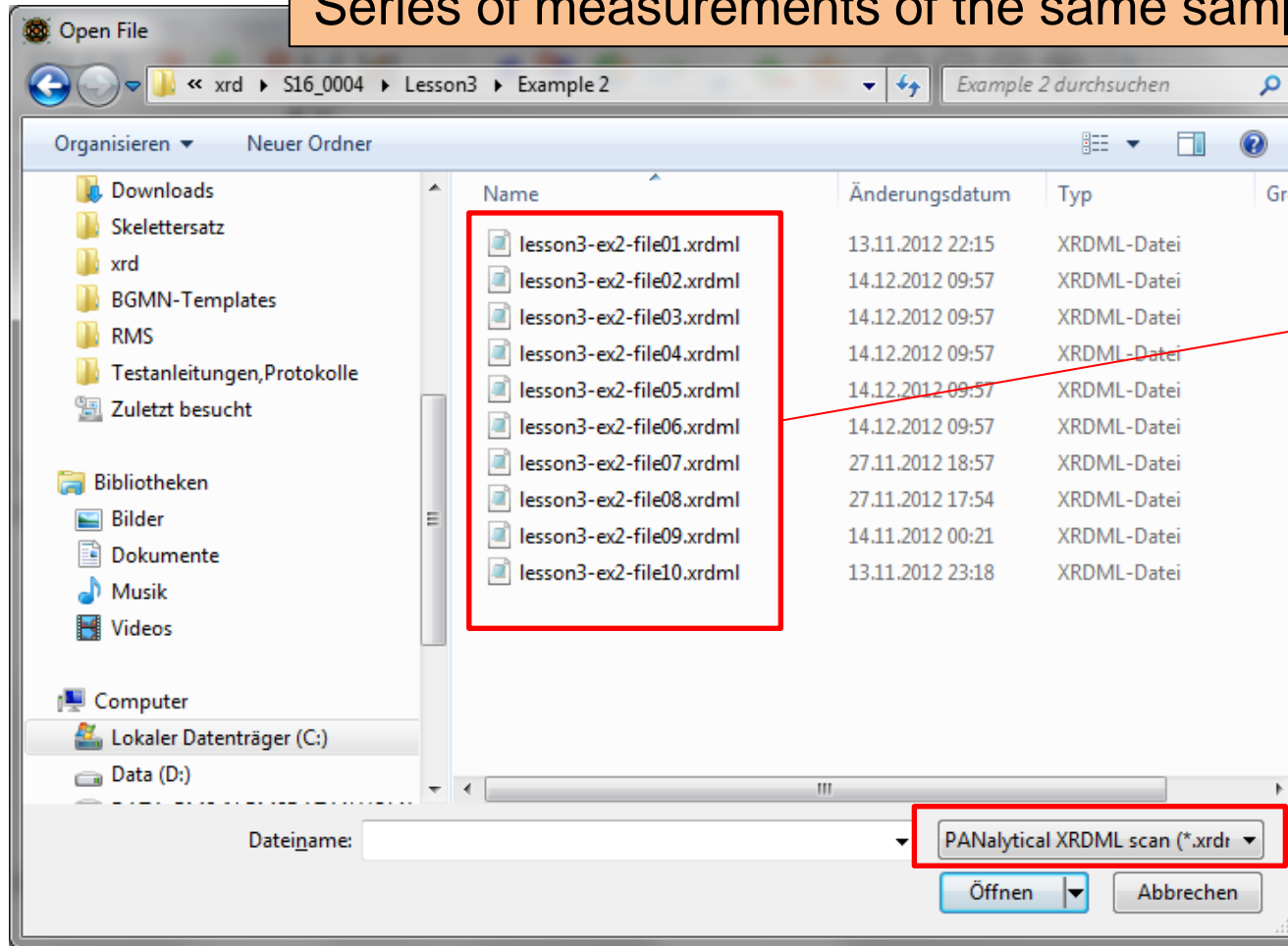


Optimized Refinement



Example 2: Batch Refinement

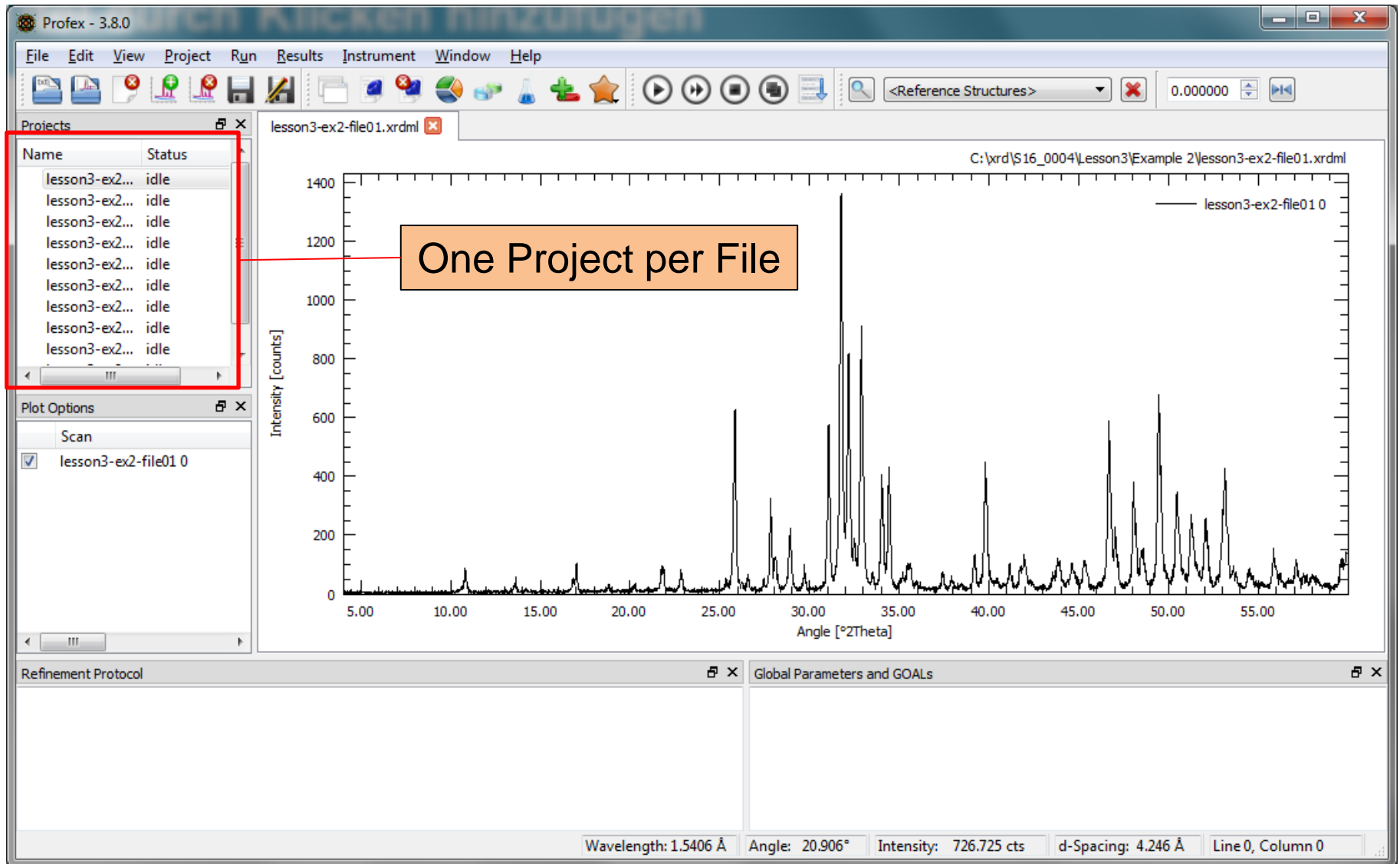
Series of measurements of the same sample



2. Select and open all files

1. Set Format

Example 2: Batch Refinement



Example 2: Batch Refinement

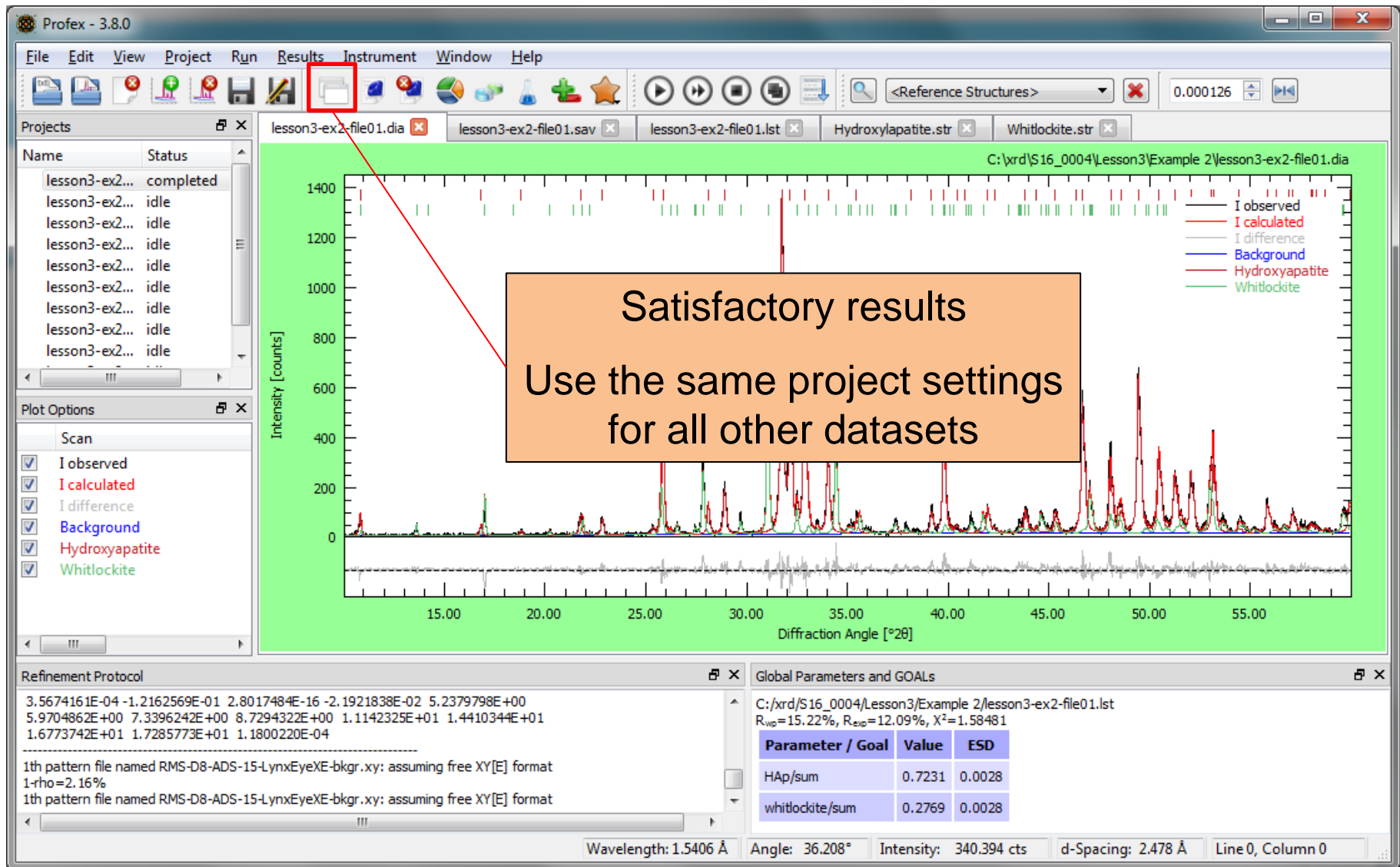
The screenshot displays the Profex 3.8.0 software interface. The main window shows a list of projects on the left, a central text area with refinement parameters, and a bottom status bar. Two red boxes highlight the 'Add' (+) and 'Run' (play) icons in the toolbar. Two orange callout boxes provide instructions: '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

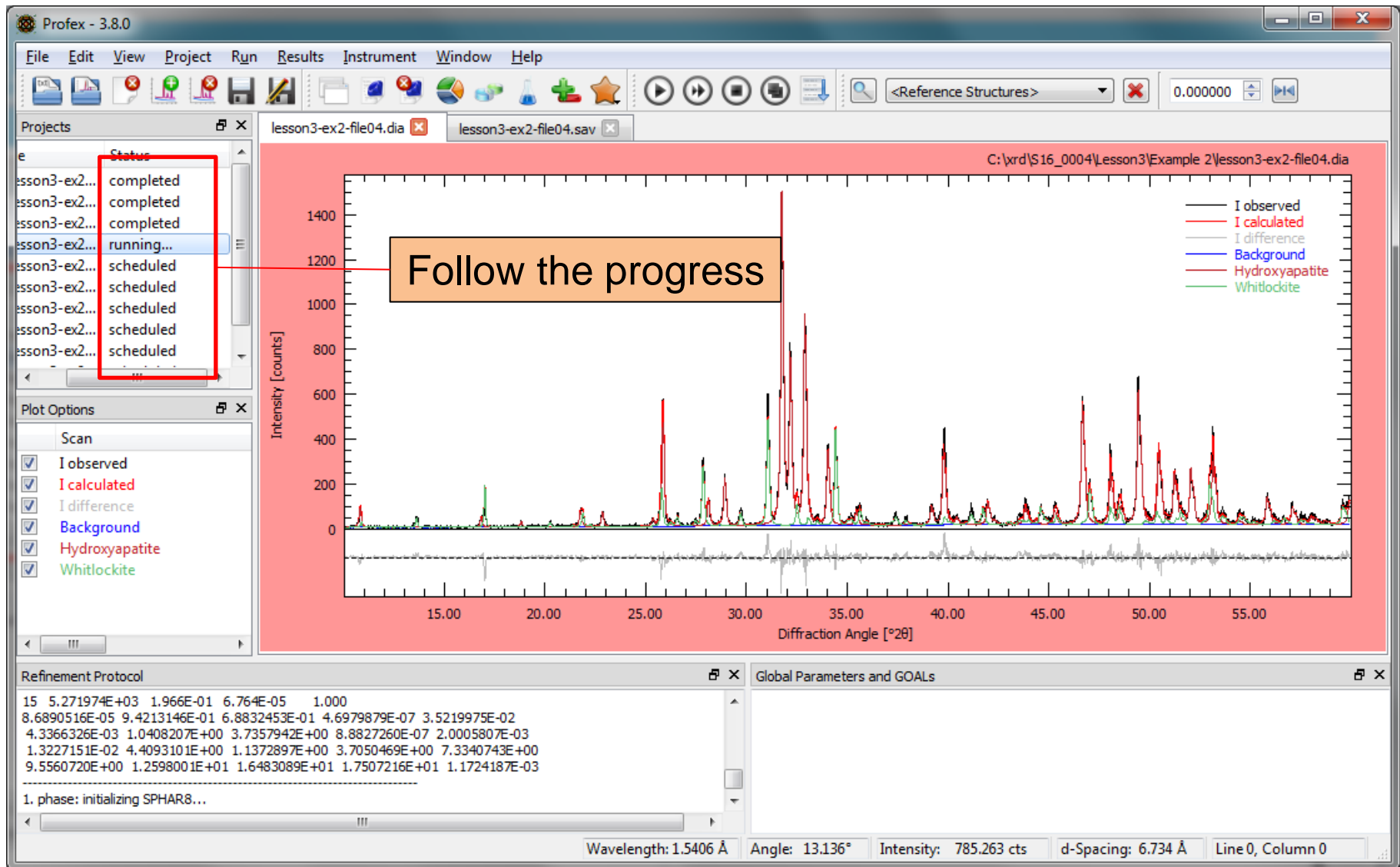
Identical control file was created

«Run Batch Refinement»
Will process all open projects

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

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

Intensity [counts]

Diffraction Angle [°2 θ]

Export results of all open projects

Refinement Protocol

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

Exported Global GOALS

The screenshot shows a Microsoft Excel window titled "results.csv - Microsoft Excel". The spreadsheet contains a table with 5 columns: A (File), B (Sample), C (Parameter / Goal), D (Value), and E (ESD). The data is sorted by the "Parameter / Goal" column. An orange callout box with the text "Sort by «Parameter/Goal»" is overlaid on the table. The status bar at the bottom indicates "Bereit" and "100 %".

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-file01.lst	lesson3-ex2-file01	whitlockite/sum	0.2769	0.0028
4	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file01.lst	lesson3-ex2-file01	Rwp	15.22	
5	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file01.lst	lesson3-ex2-file01	Rexp	12.09	
6	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file01.lst	lesson3-ex2-file01	Chi2	1.5848	
7	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file02.lst	lesson3-ex2-file02	HAp/sum	0.7242	0.0027
8	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file02.lst	lesson3-ex2-file02	whitlockite/sum	0.2758	0.0027
9	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file02.lst	lesson3-ex2-file02	Rwp	14.92	
10	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file02.lst	lesson3-ex2-file02	Rexp	12.02	
11	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file02.lst	lesson3-ex2-file02	Chi2	1.5407	
12	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file03.lst	lesson3-ex2-file03	HAp/sum	0.725	0.0028
13	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file03.lst	lesson3-ex2-file03	whitlockite/sum	0.275	0.0028
14	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file03.lst	lesson3-ex2-file03	Rwp	15.16	
15	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file03.lst	lesson3-ex2-file03	Rexp	12.04	
16	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file03.lst	lesson3-ex2-file03	Chi2	1.5854	
17	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file04.lst	lesson3-ex2-file04	HAp/sum	0.7196	0.0027
18	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file04.lst	lesson3-ex2-file04	whitlockite/sum	0.2804	0.0027
19	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file04.lst	lesson3-ex2-file04	Rwp	14.8	
20	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file04.lst	lesson3-ex2-file04	Rexp	12.01	
21	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file04.lst	lesson3-ex2-file04	Chi2	1.5186	
22	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file05.lst	lesson3-ex2-file05	HAp/sum	0.7213	0.0027
23	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file05.lst	lesson3-ex2-file05	whitlockite/sum	0.2787	0.0027
24	C:/xrd/S16_0004/Lesson3/Example 2\lesson3-ex2-file05.lst	lesson3-ex2-file05	Rwp	14.94	
25	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:

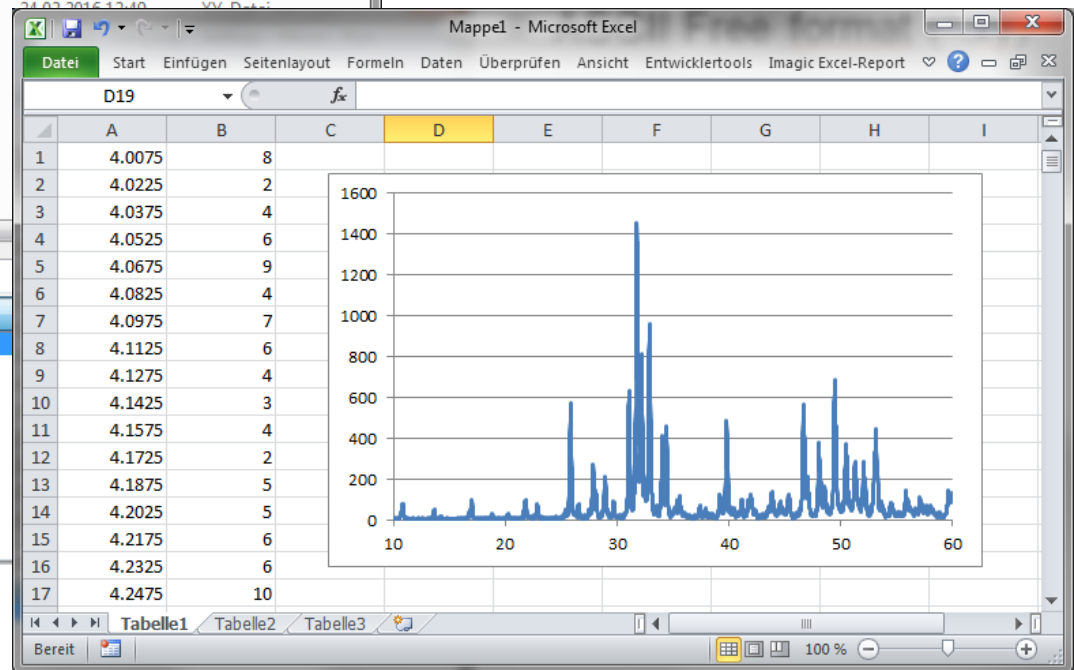
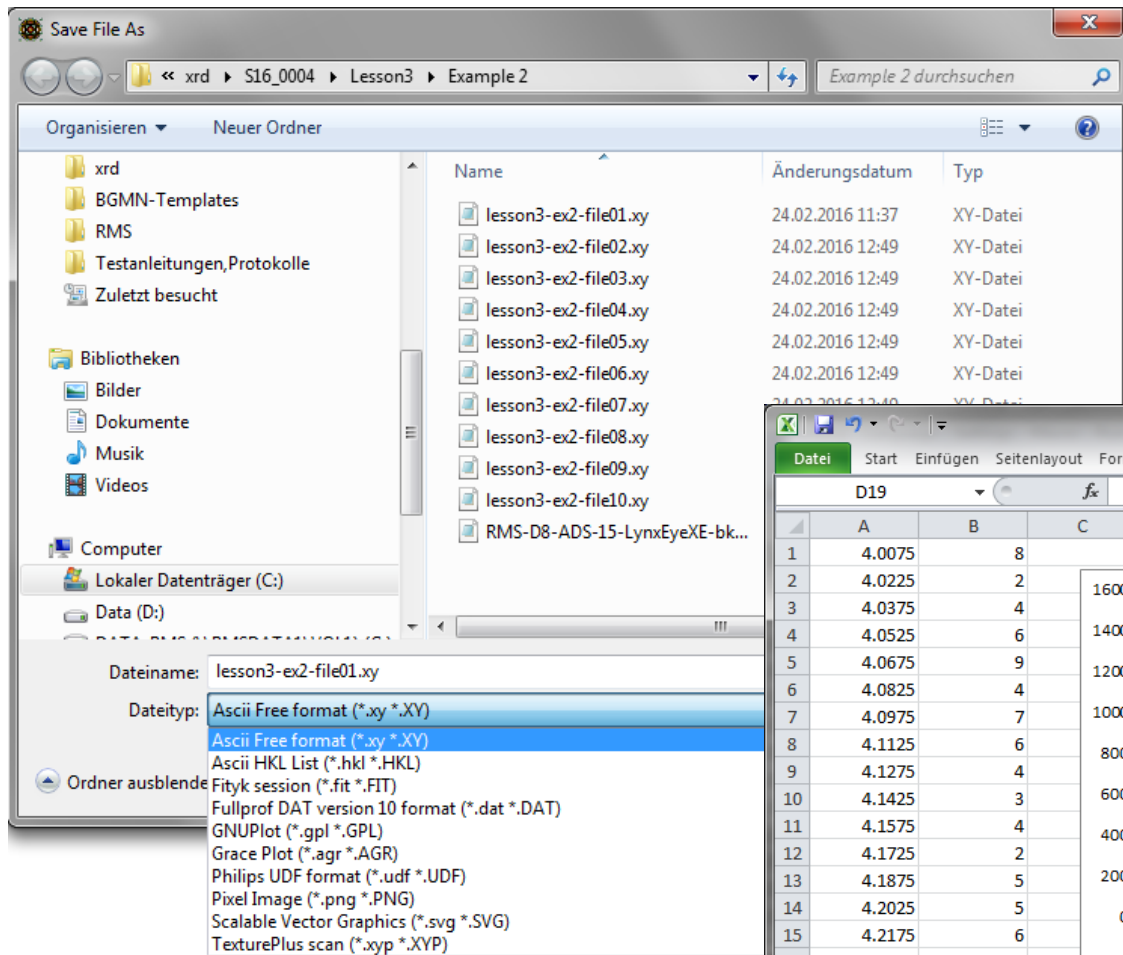
Parameter / Goal	Value	ESD
HAp/sum	0.7231	0.0028
whitlockite/sum	0.2769	0.0028

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.

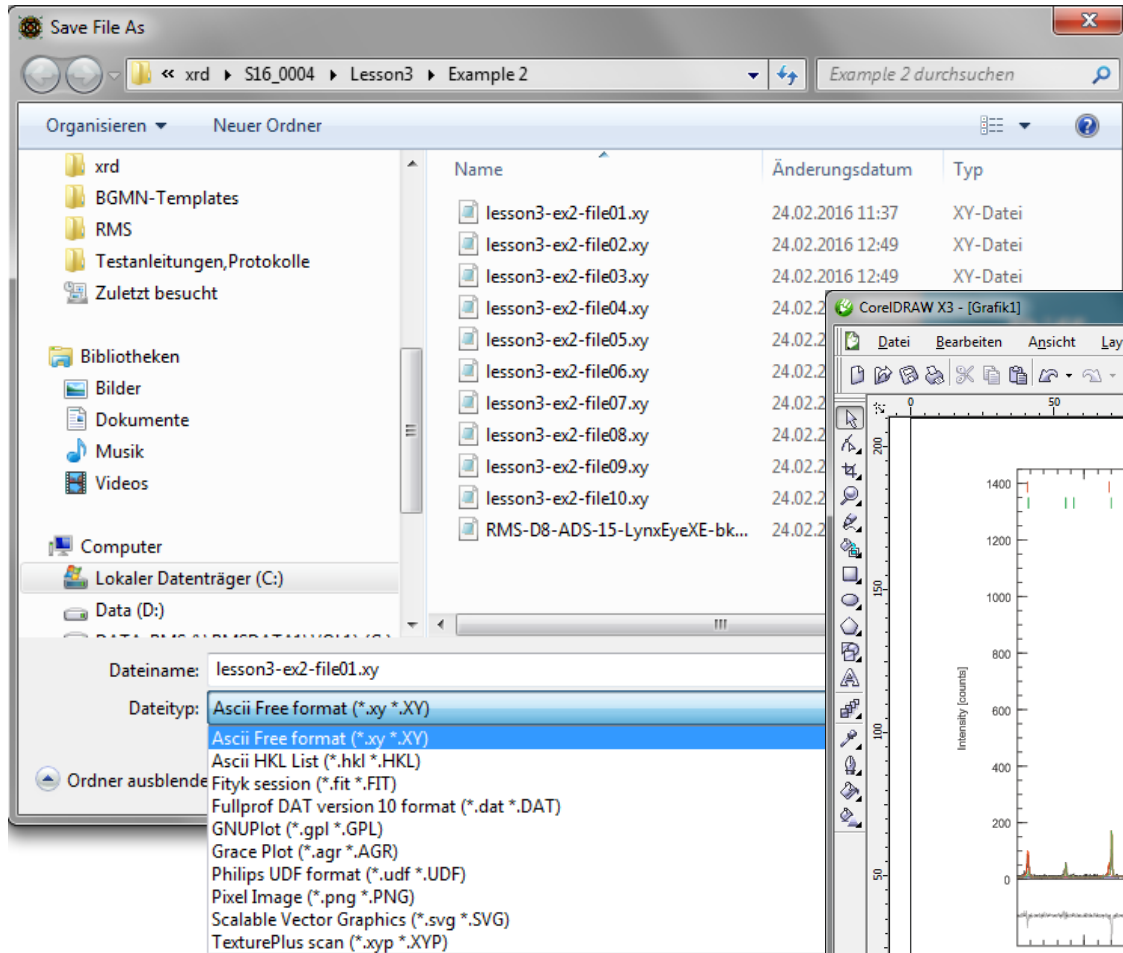
Diffraction Data Formats

ASCII Free format (*.xy)

for import in
Excel, Origin, etc.

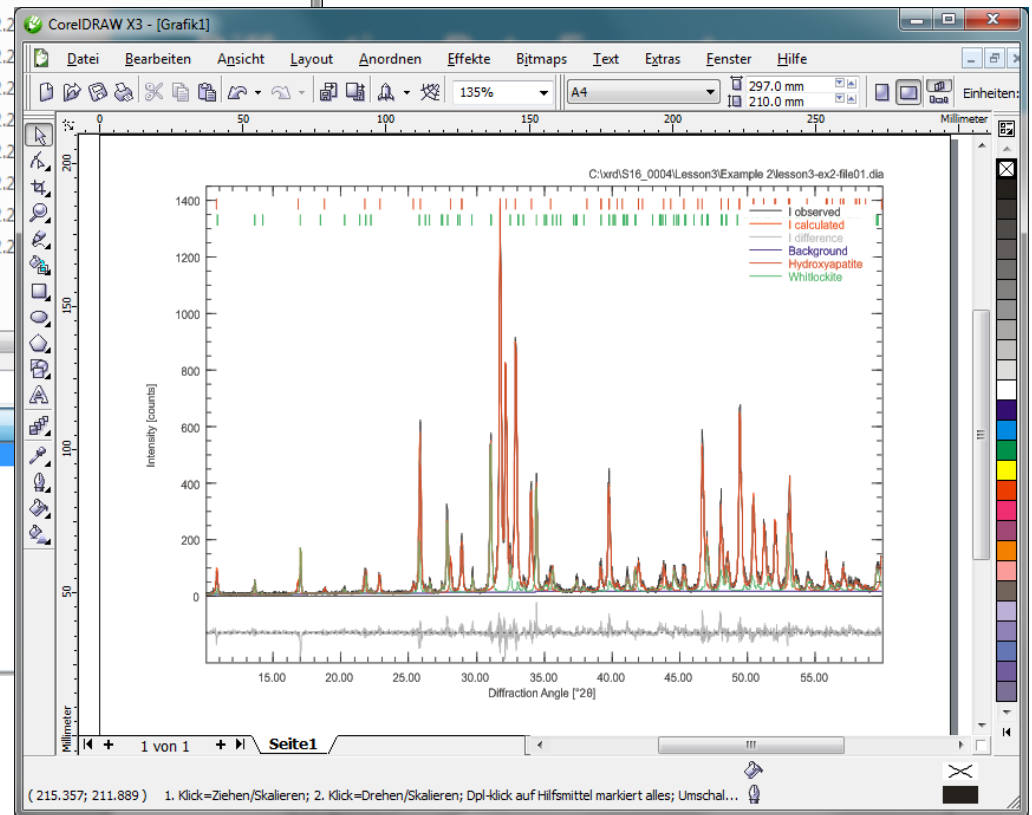


Diffraction Data Formats

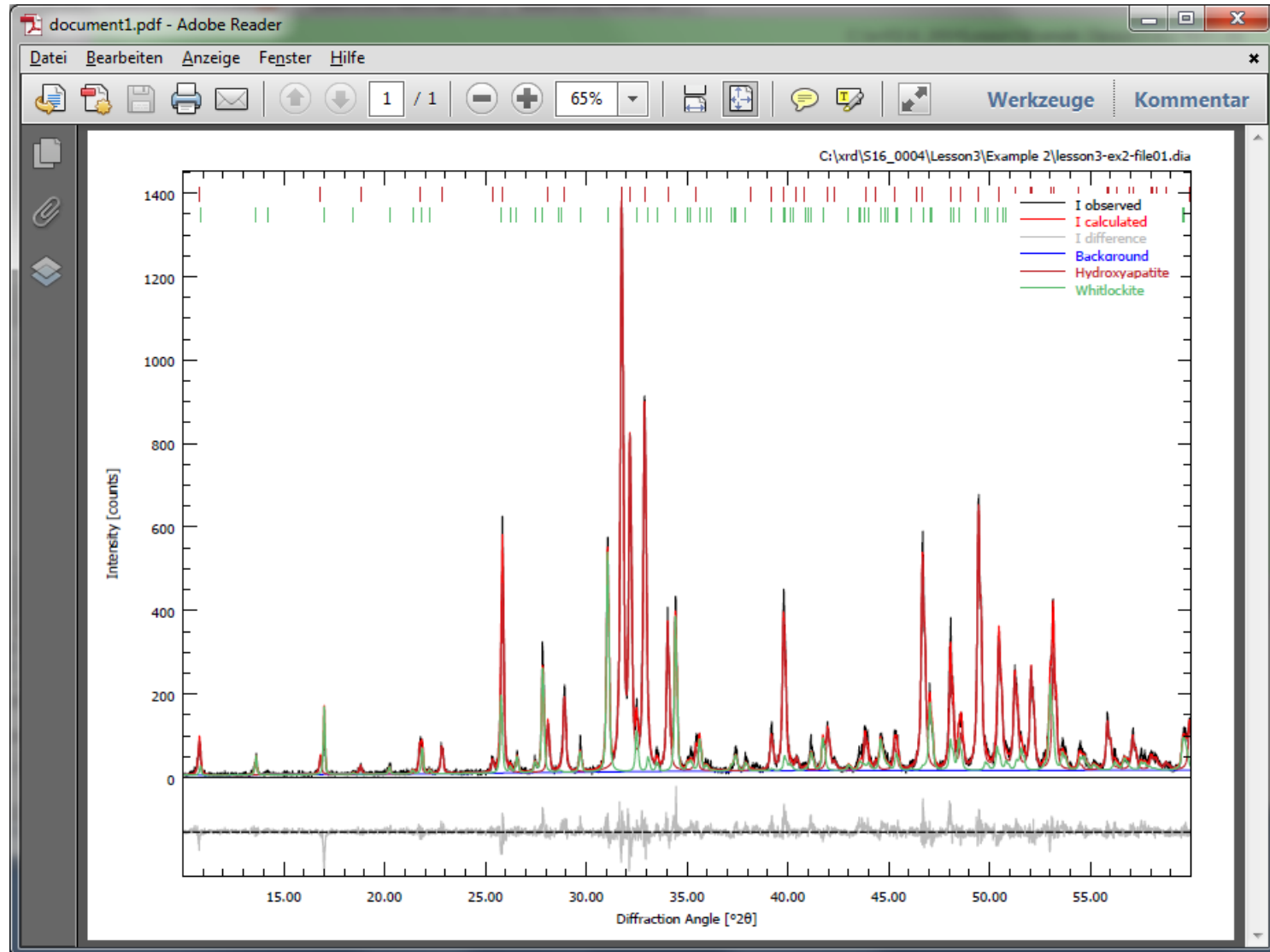


Scalable Vector Graphics (*.svg)

for import in Illustrator, CoreIDRAW, Inkscape etc.



Diffraction Data Formats



- ▶ More «Behind the Scenes» information in «Lesson 6: Crystal Structures»



PROFEX

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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...](#)