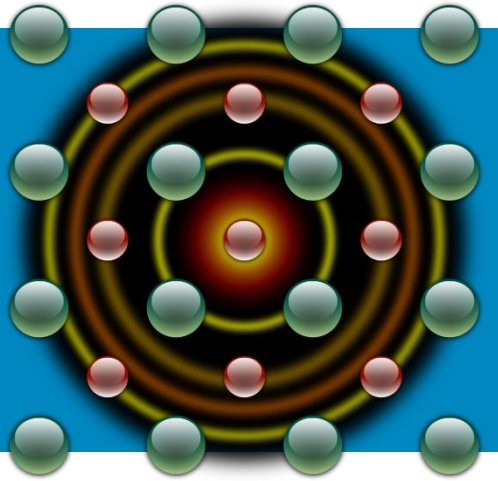
Lesson 6
Profex

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

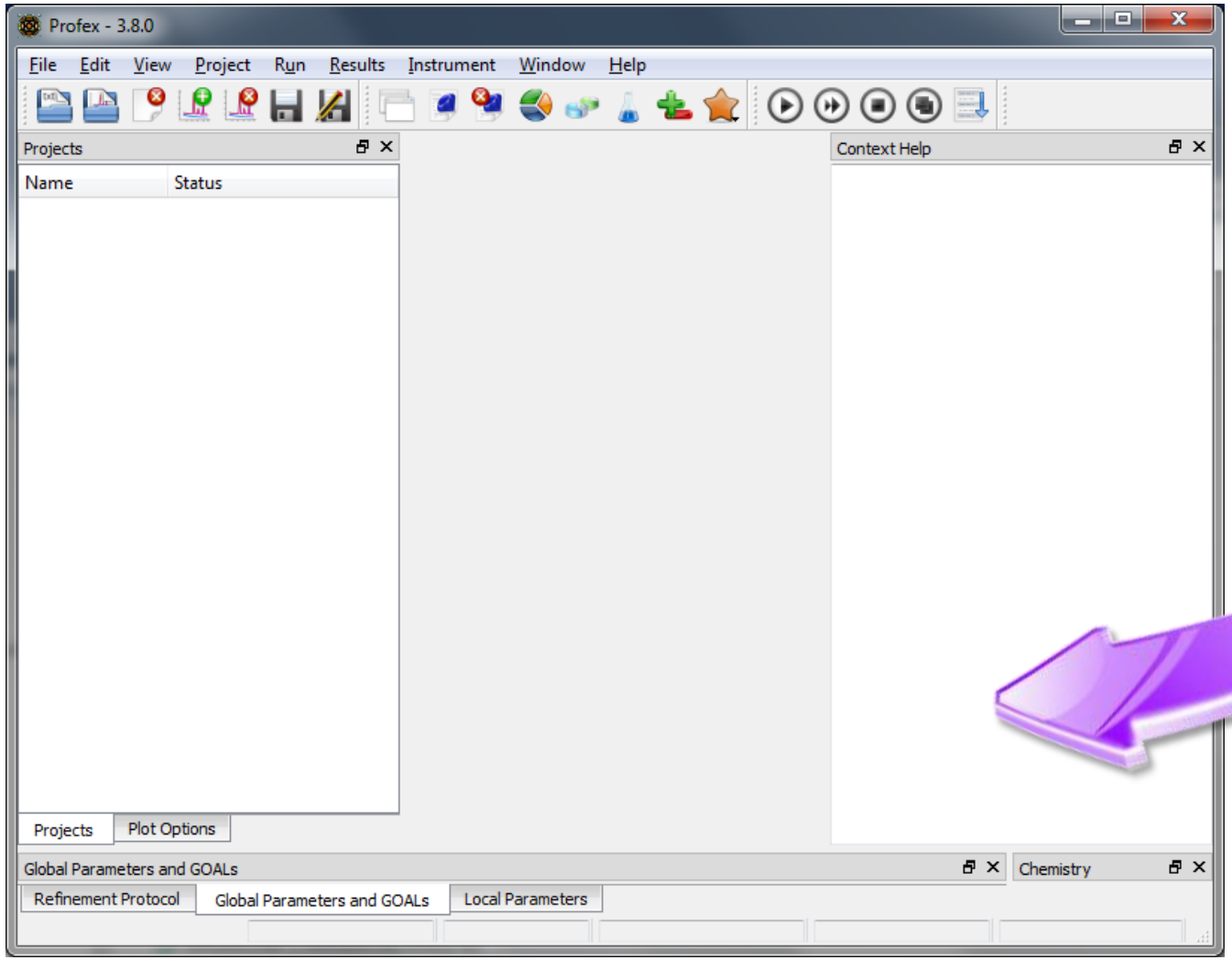
2006: Major rewrite

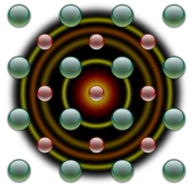
Support for Windows

2012: Support for BGMN Rietveld Backend added

2014: Support for Mac OS X

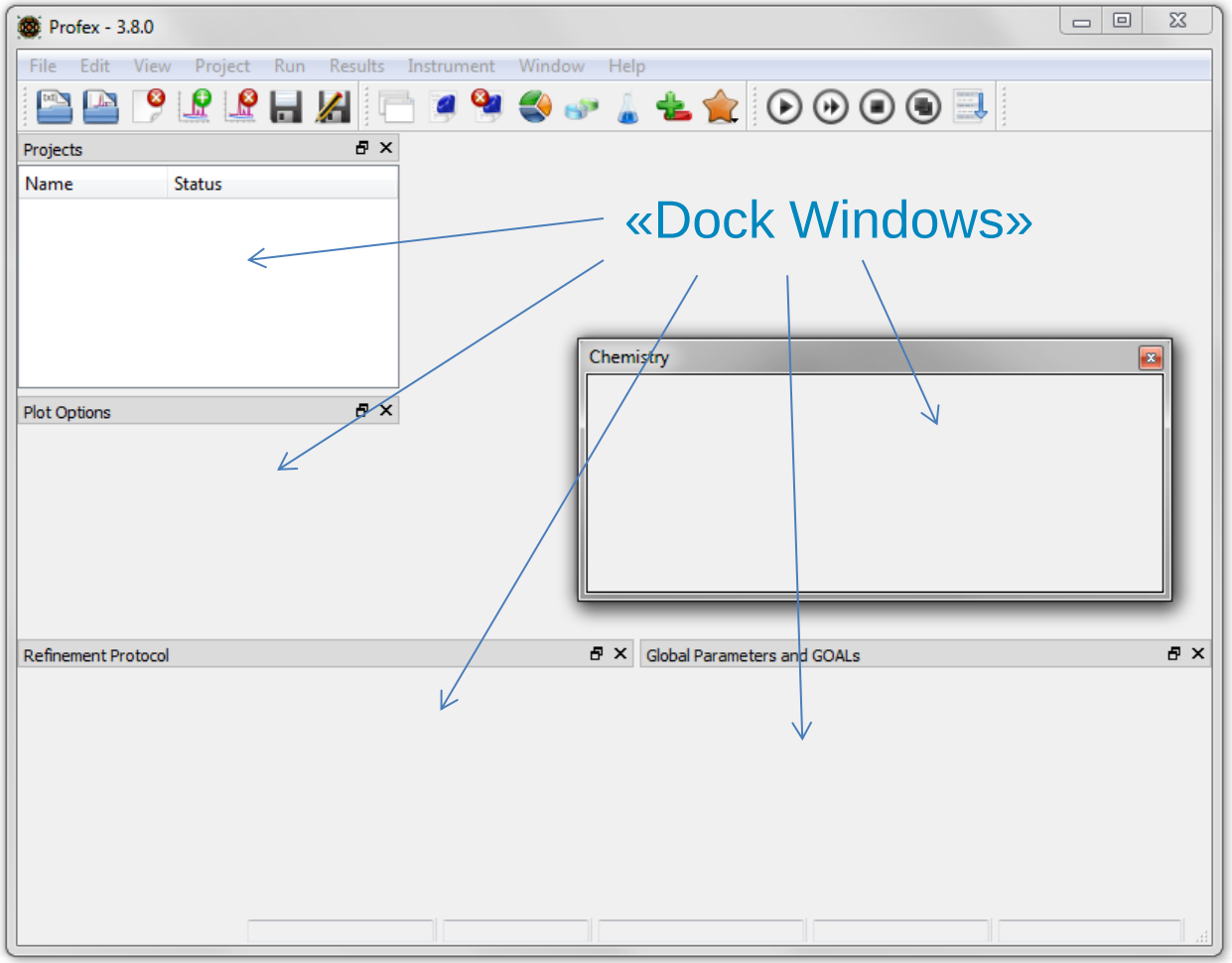
First Use





Profex

First Use



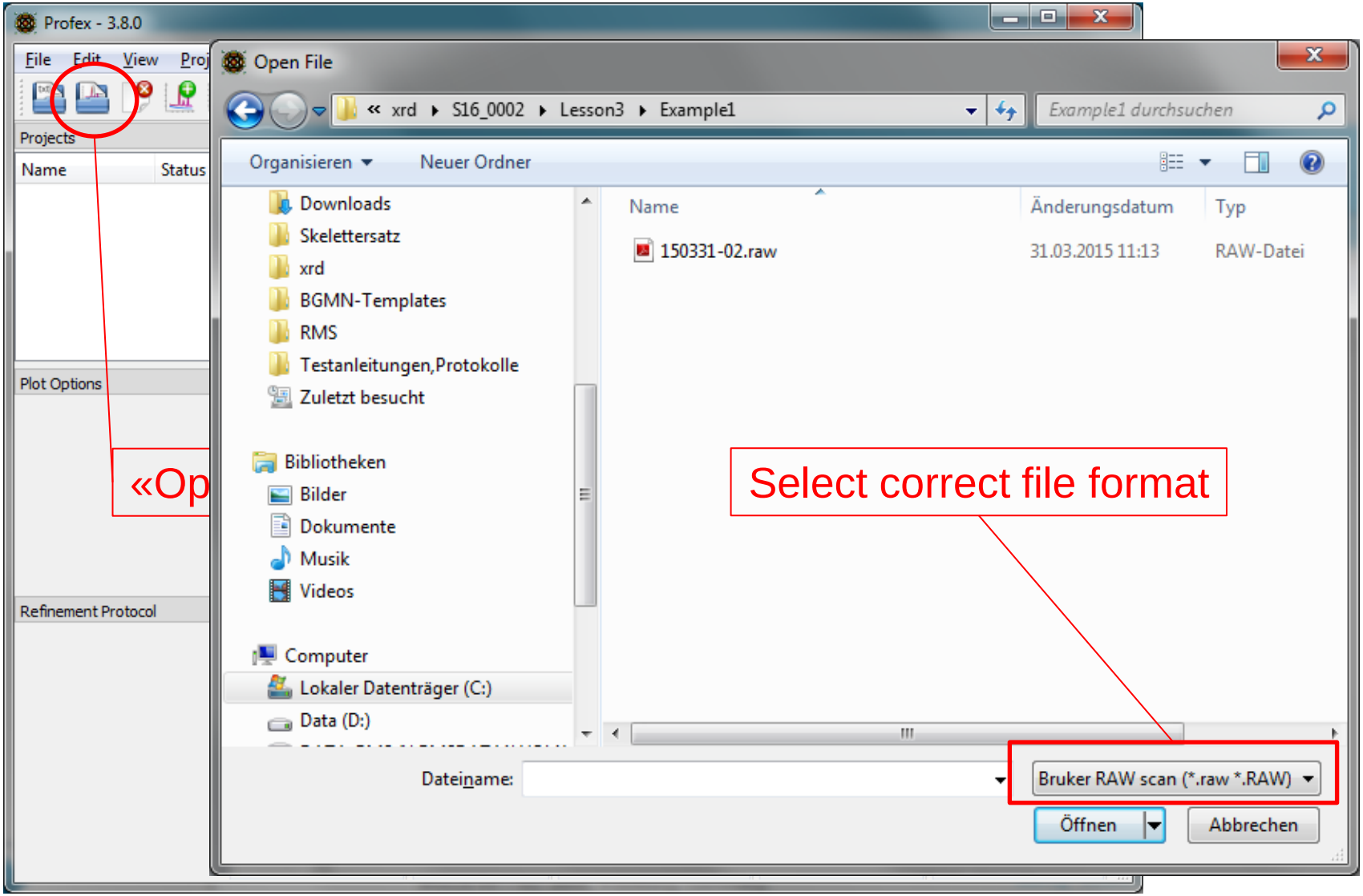
Can be re-arranged (drag & drop)

Stacked

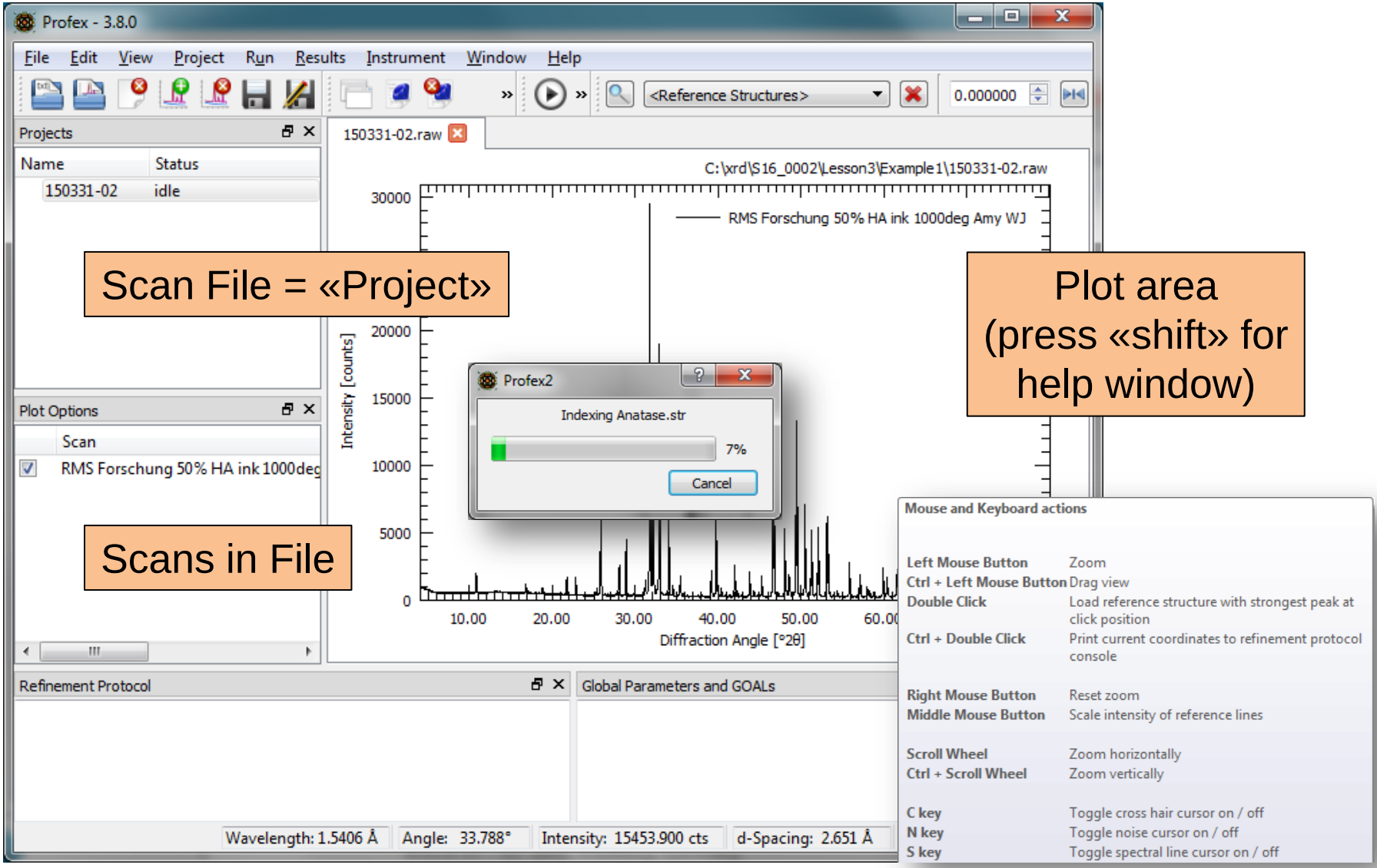
Floating

Closed (opened from «Window» menu)

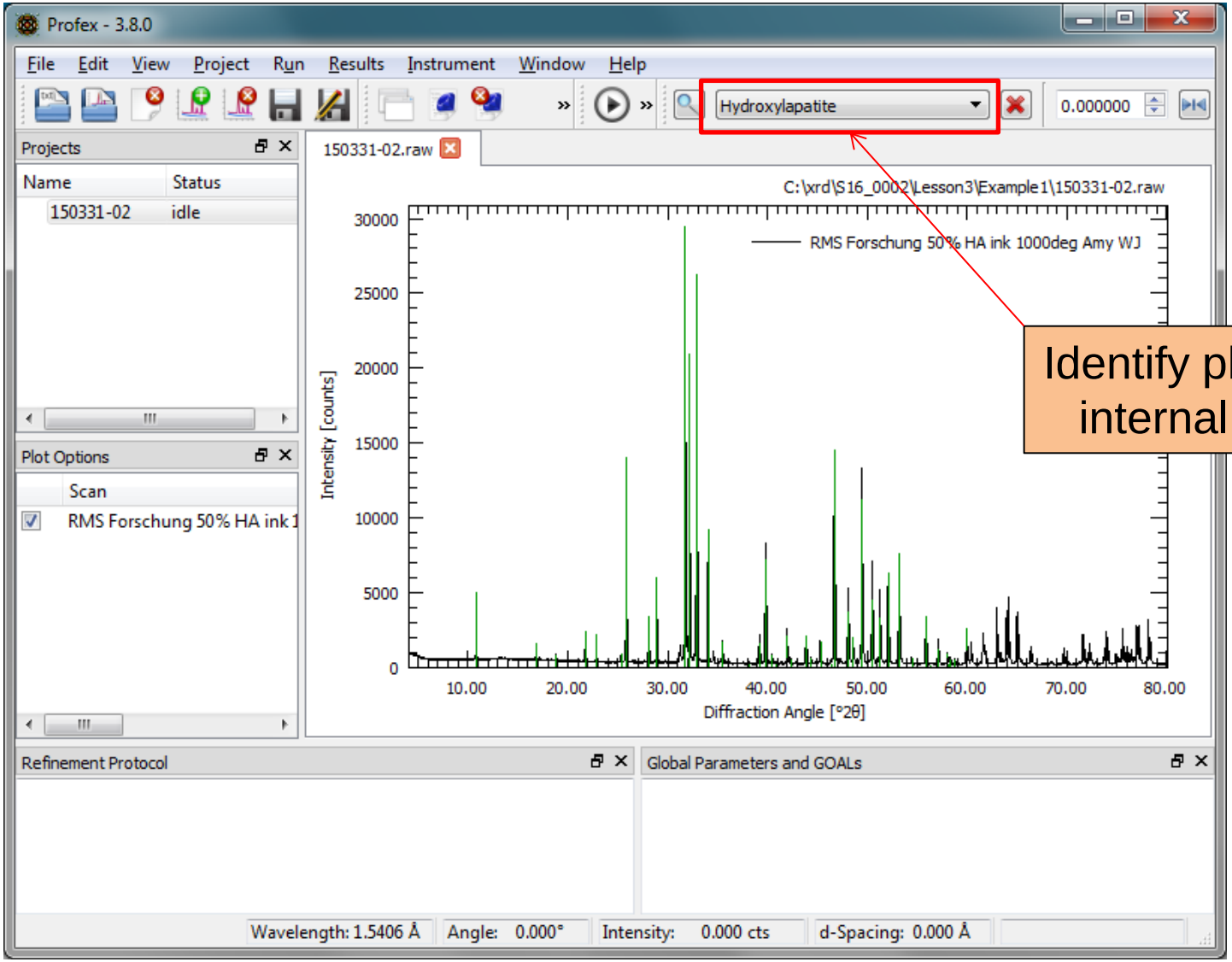
Load Scan File



First Use: Example 1

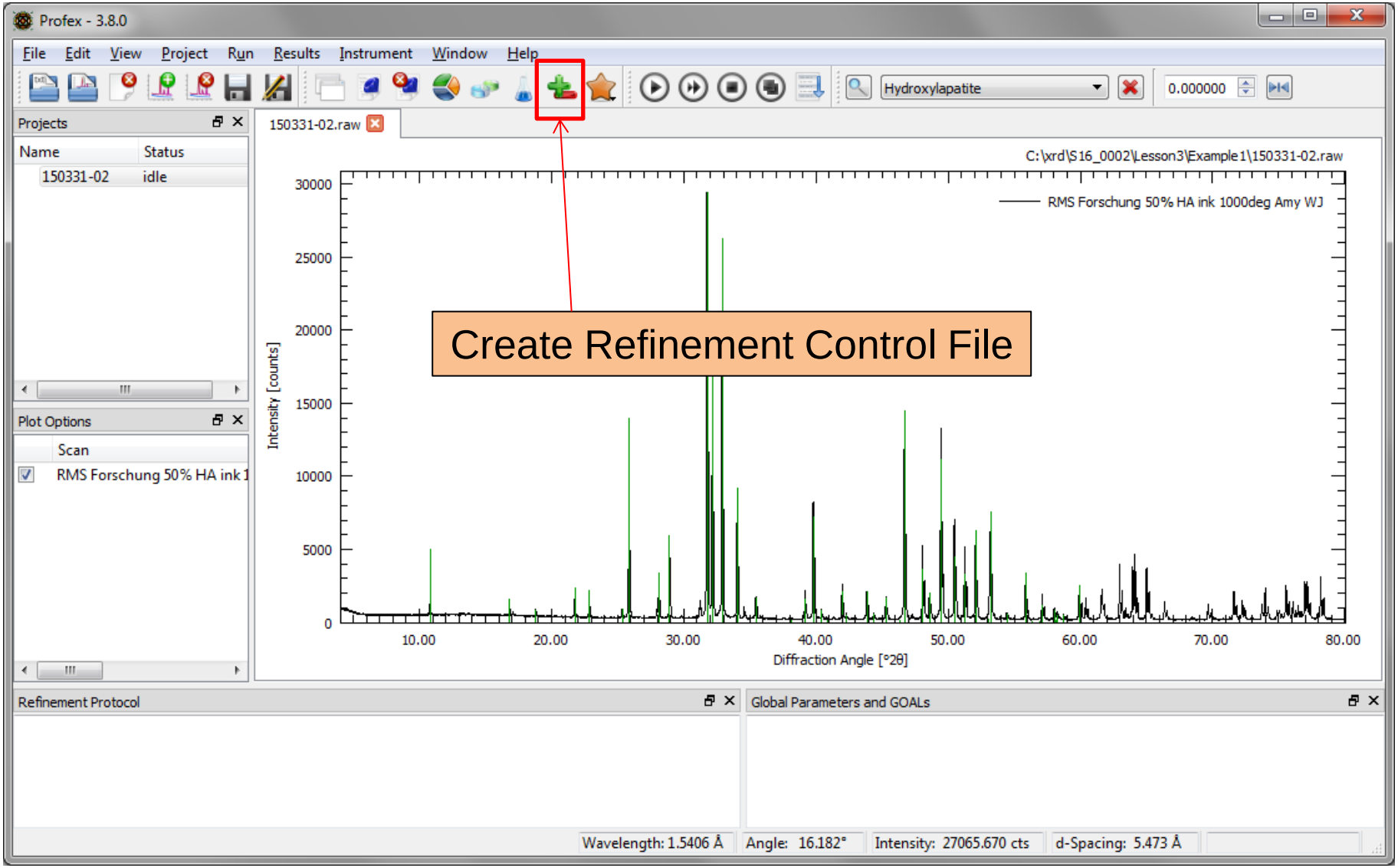


First Use: Example 1

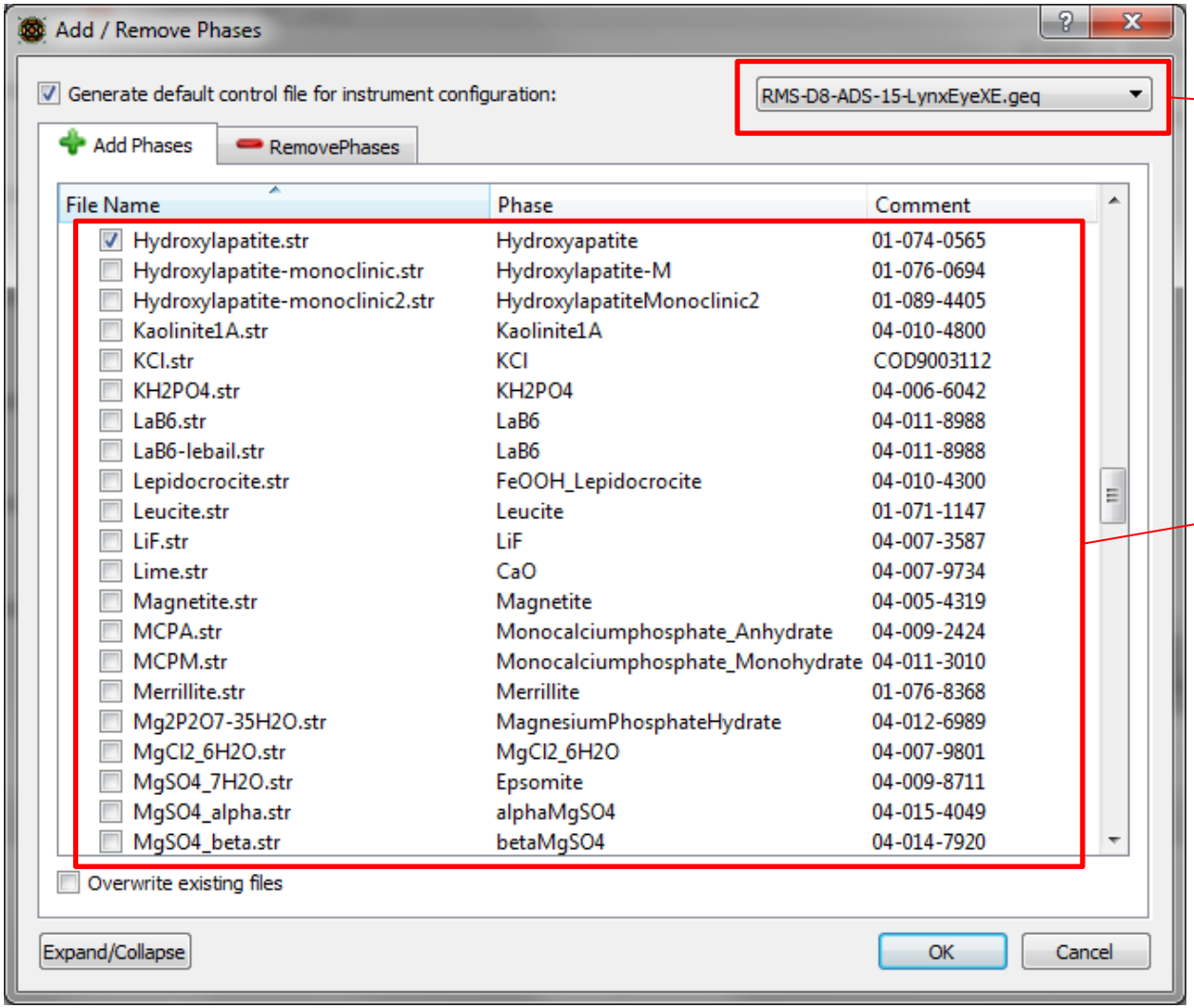


Identify phases from internal database

First Use: Example 1



First Use: Example 1

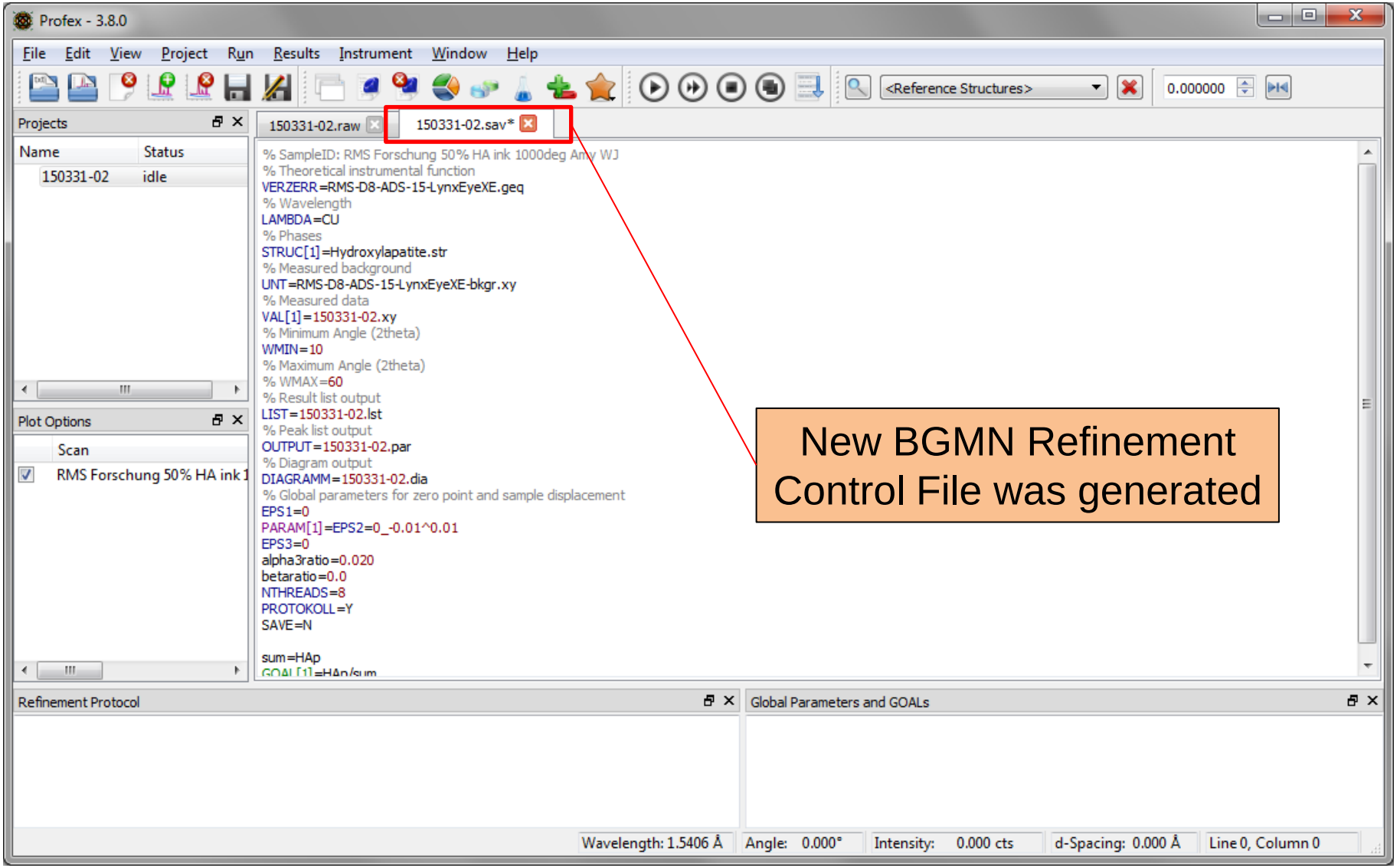


Choose correct instrument configuration

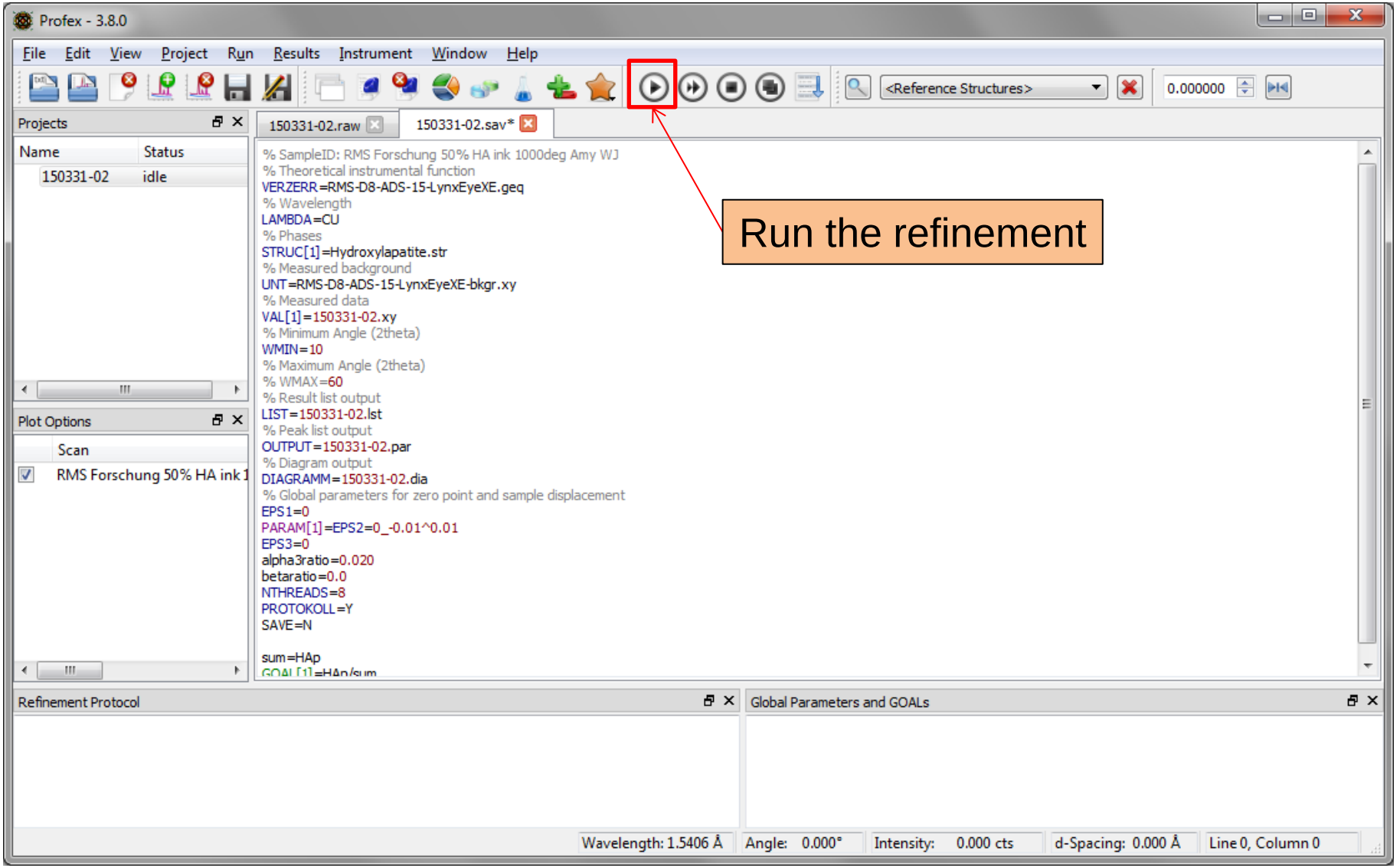
Select phases

(HAp is pre-selected)

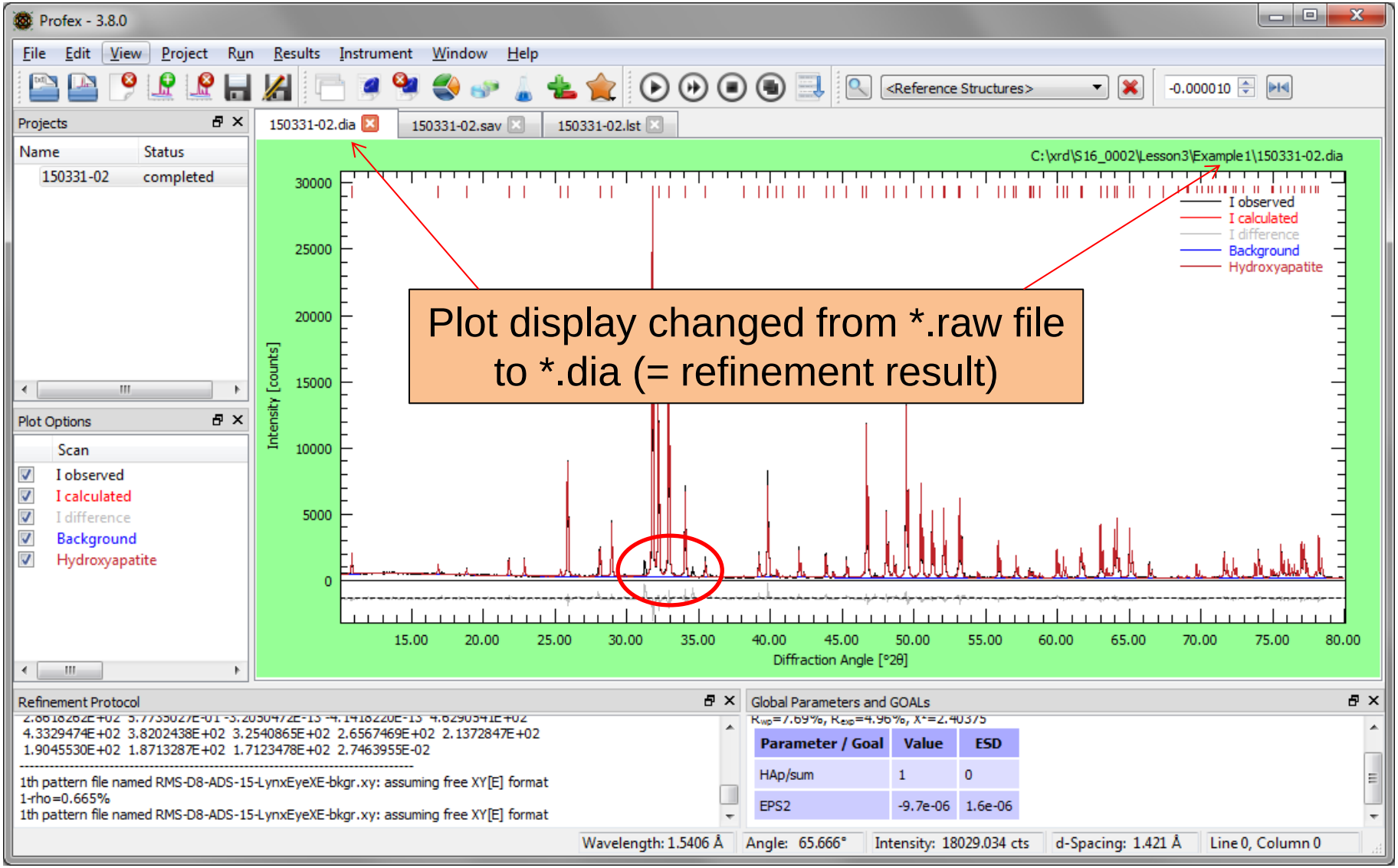
First Use: Example 1



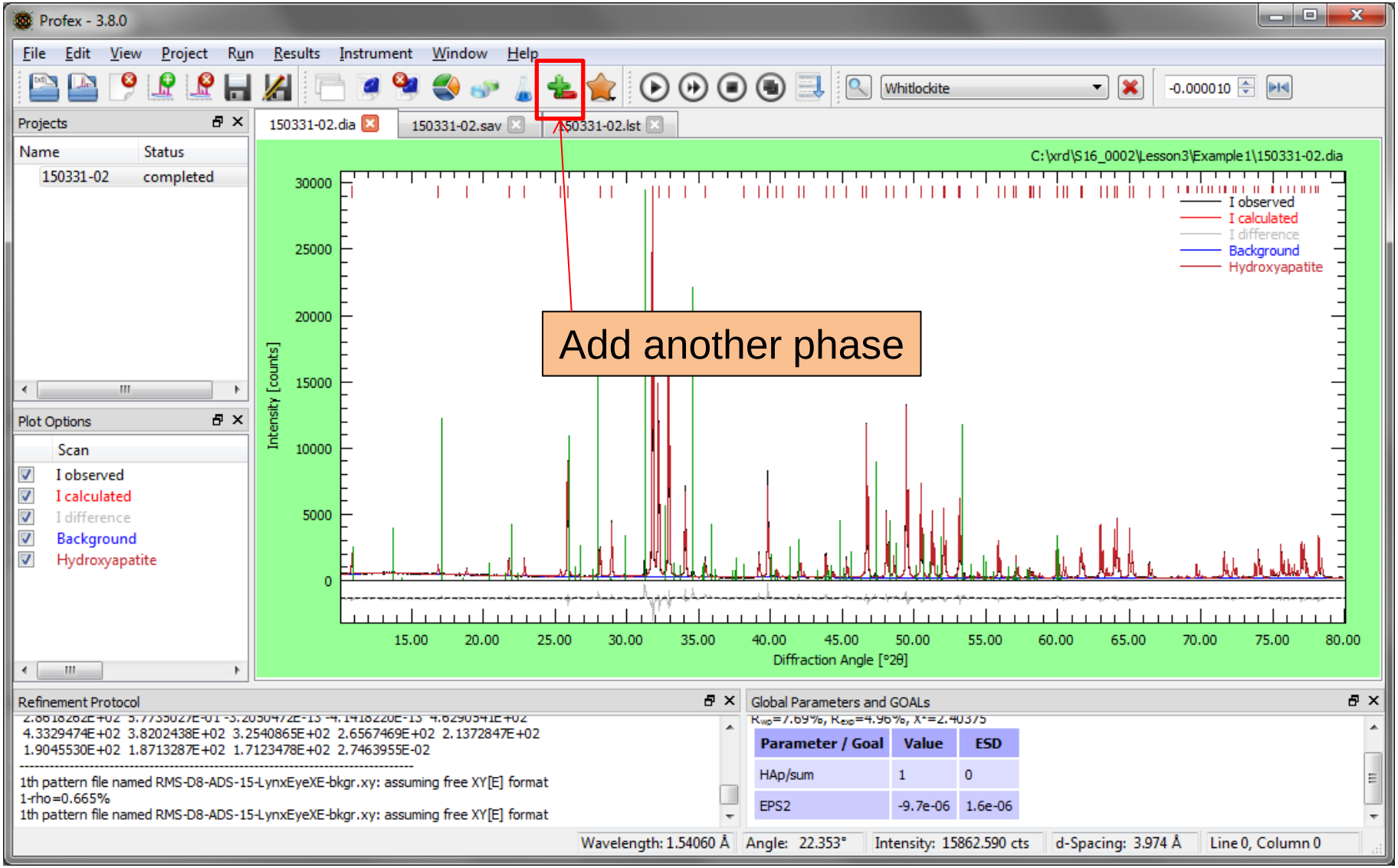
First Use: Example 1



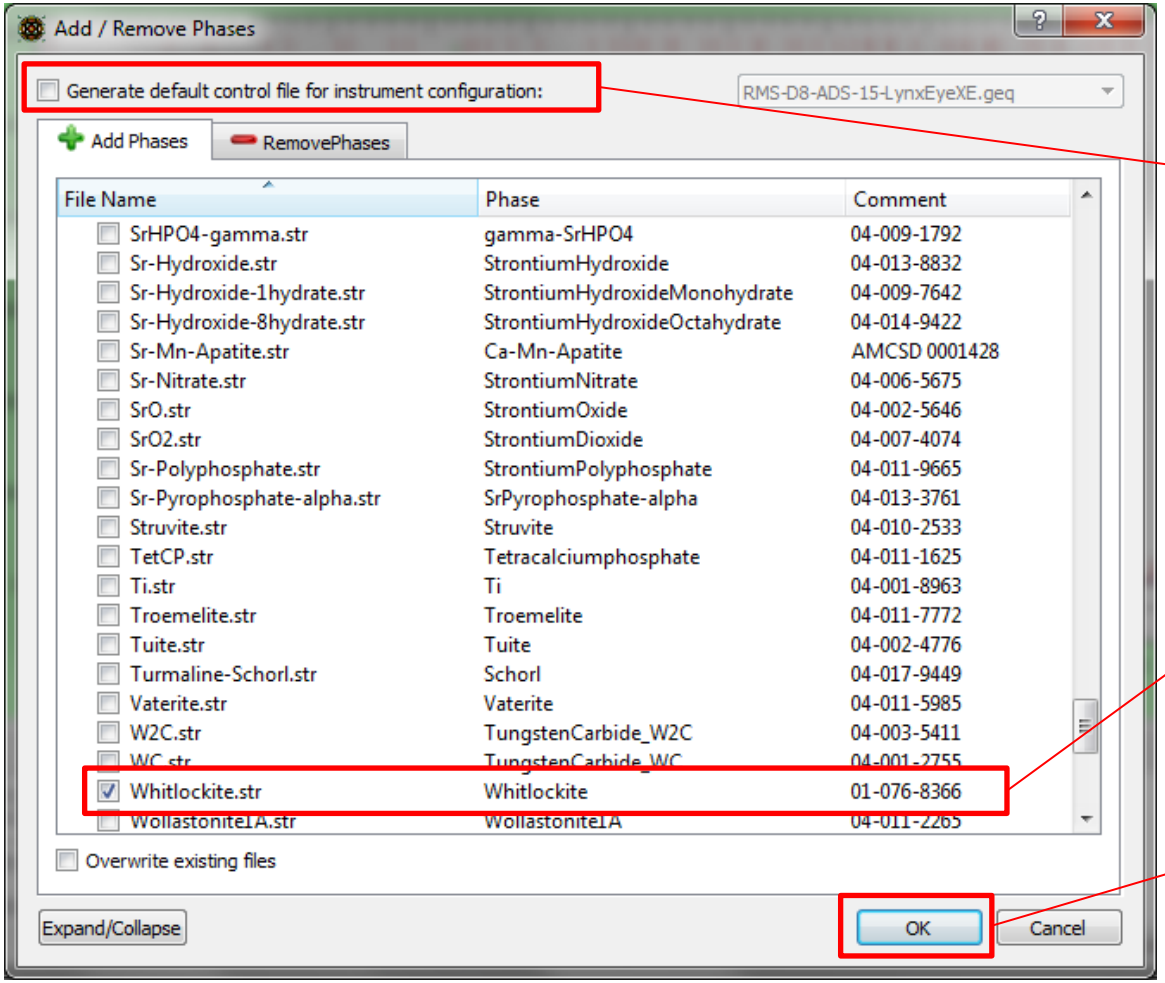
First Use: Example 1



First Use: Example 1



First Use: Example 1

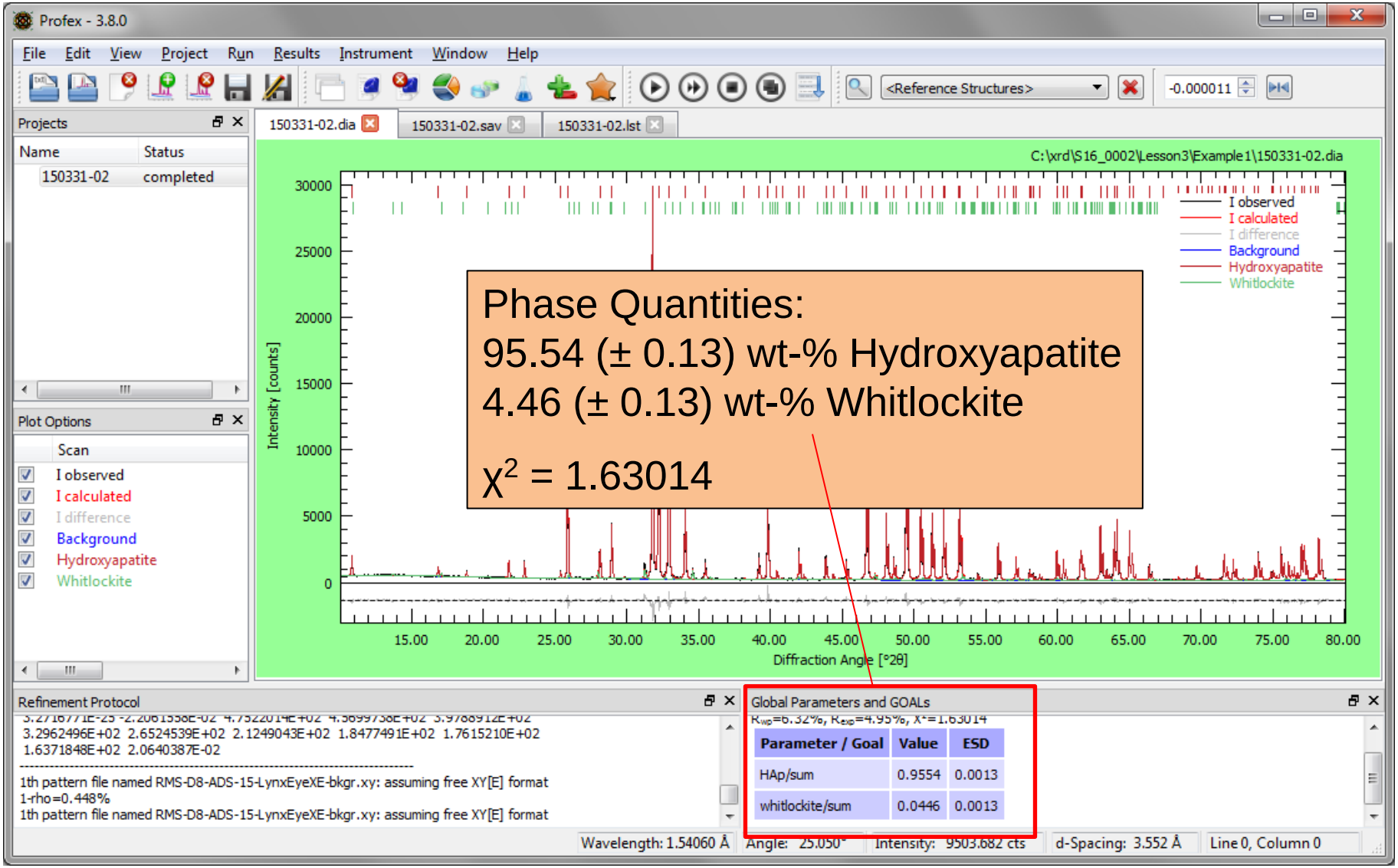


Control file already exists, **don't** generate a new default file

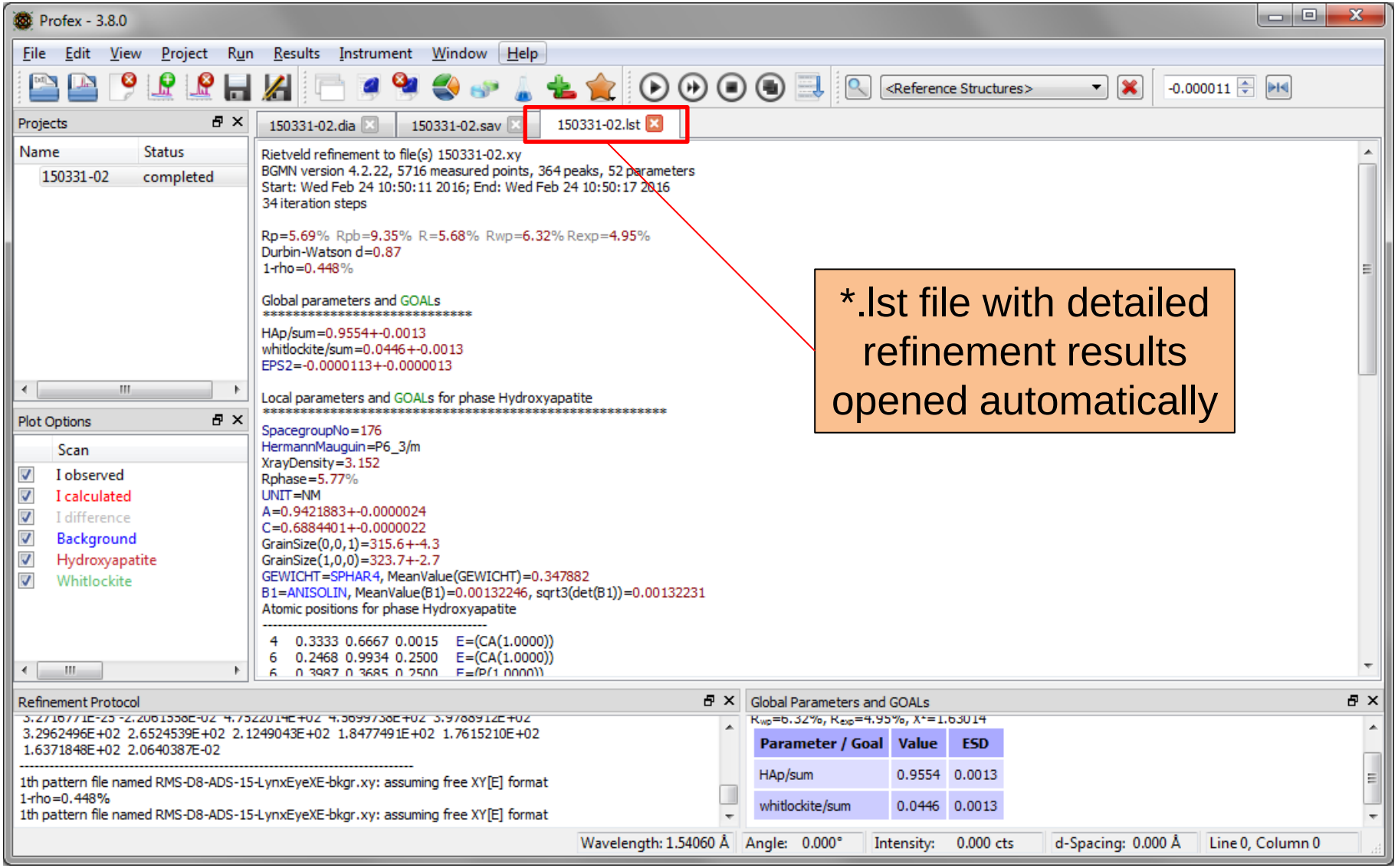
Select Whitlockite

Click «OK» and re-run the refinement

First Use: Example 1



First Use: Example 1

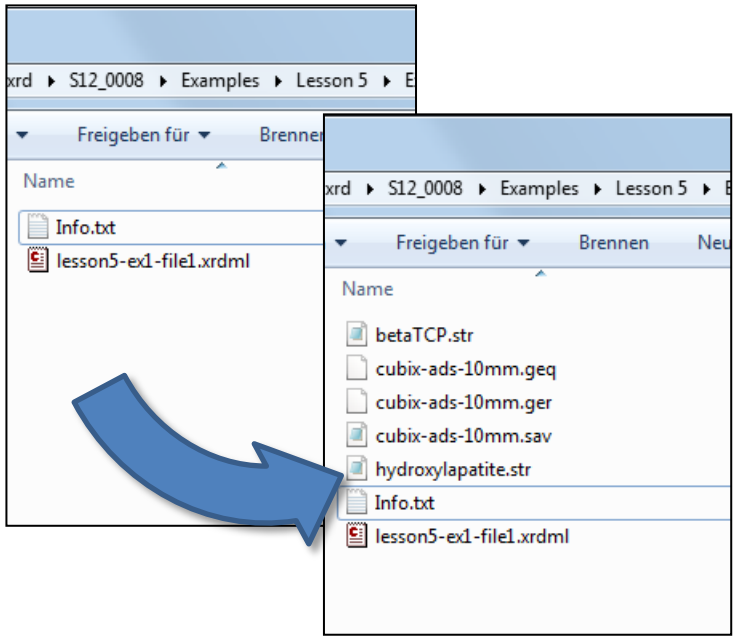


*.lst file with detailed refinement results opened automatically

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]=B1global=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

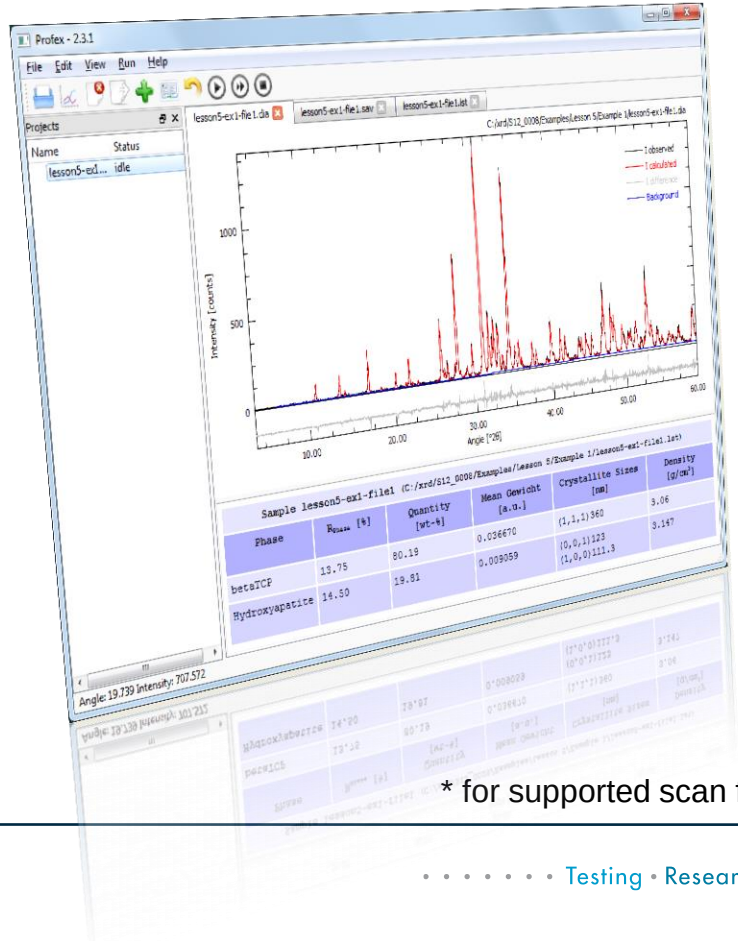
Automatic file names of output files

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)

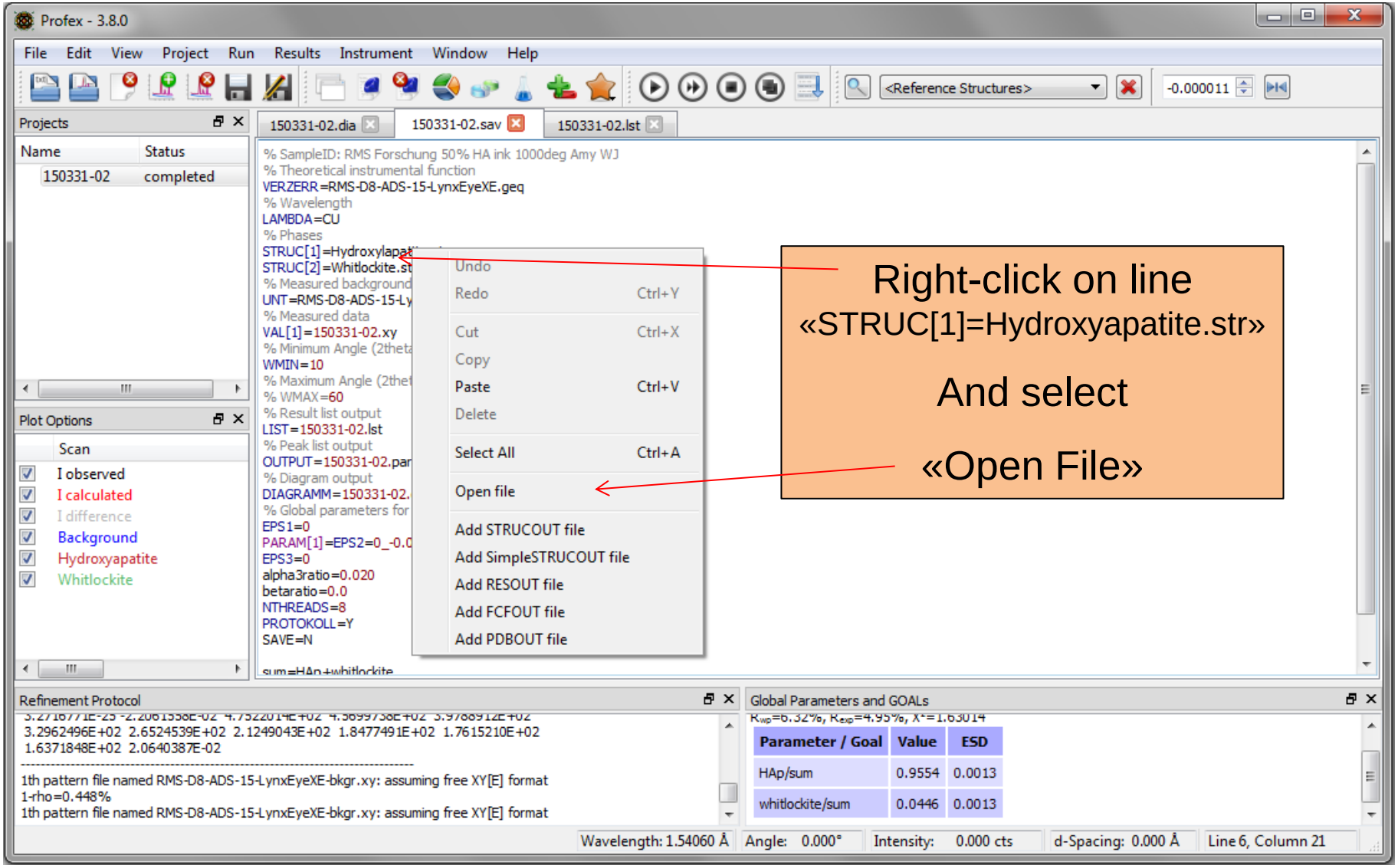
Advantages:

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

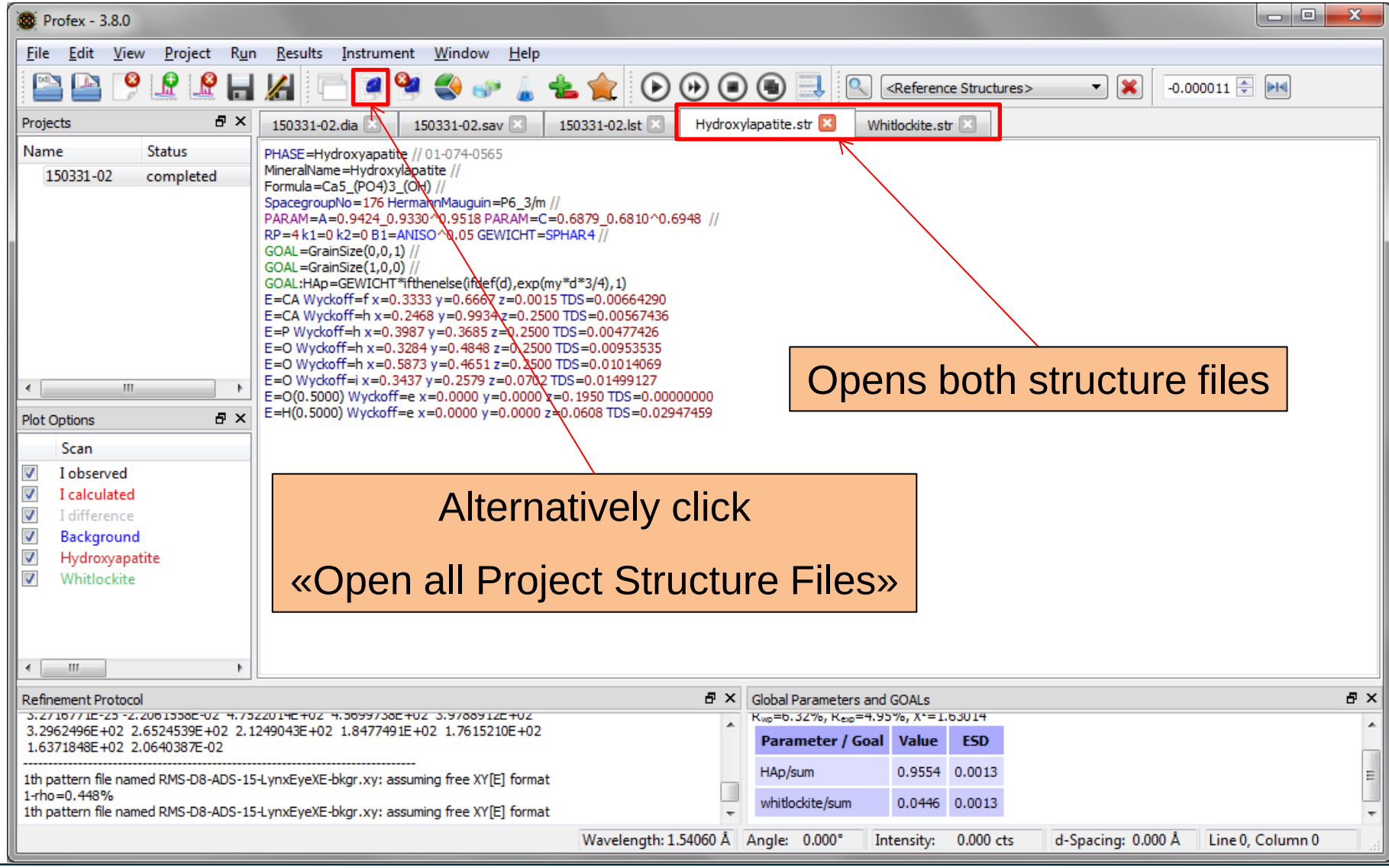
Disadvantages:

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

Optimizing the Refinement



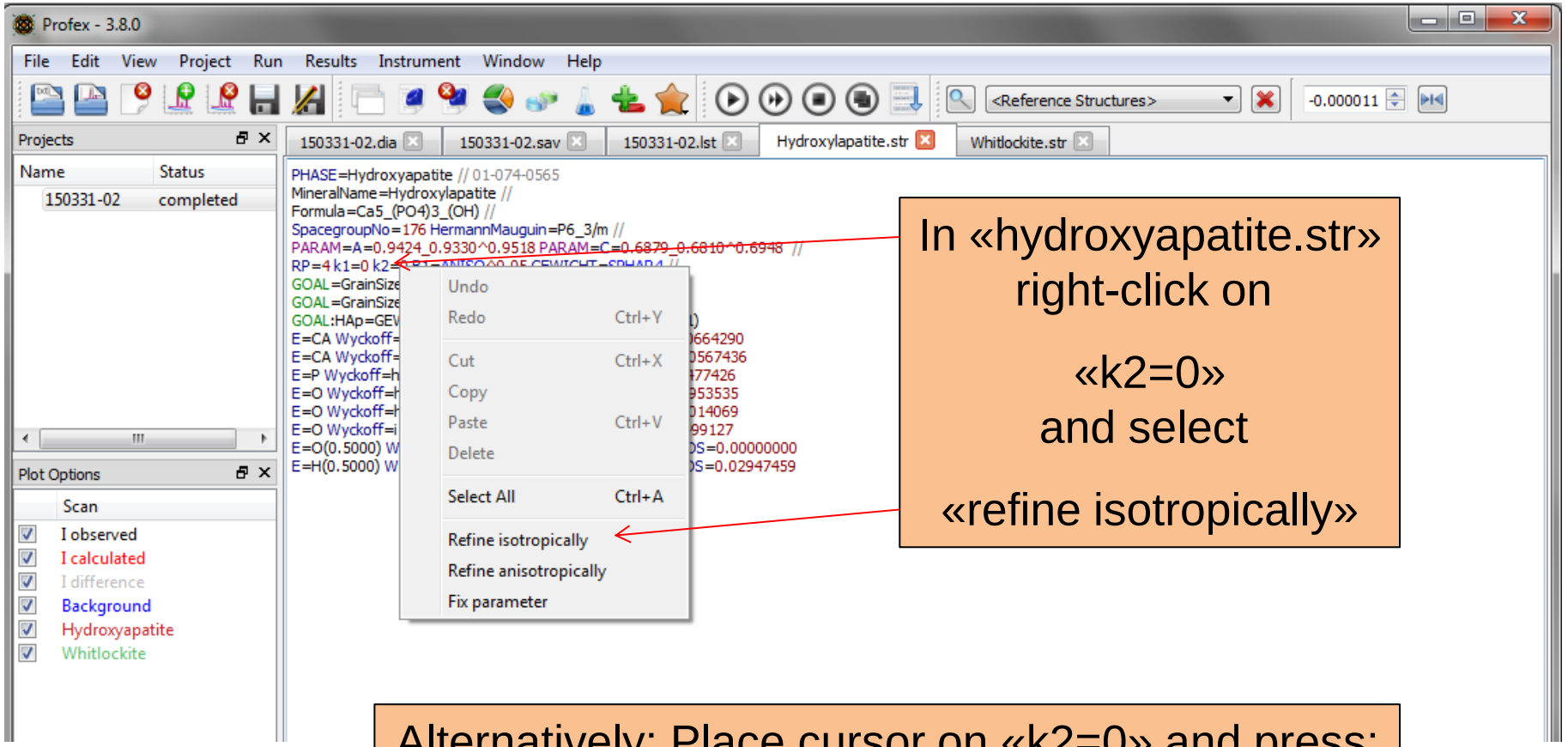
Optimizing the Refinement



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



In «hydroxyapatite.str» right-click on

«k2=0» and select

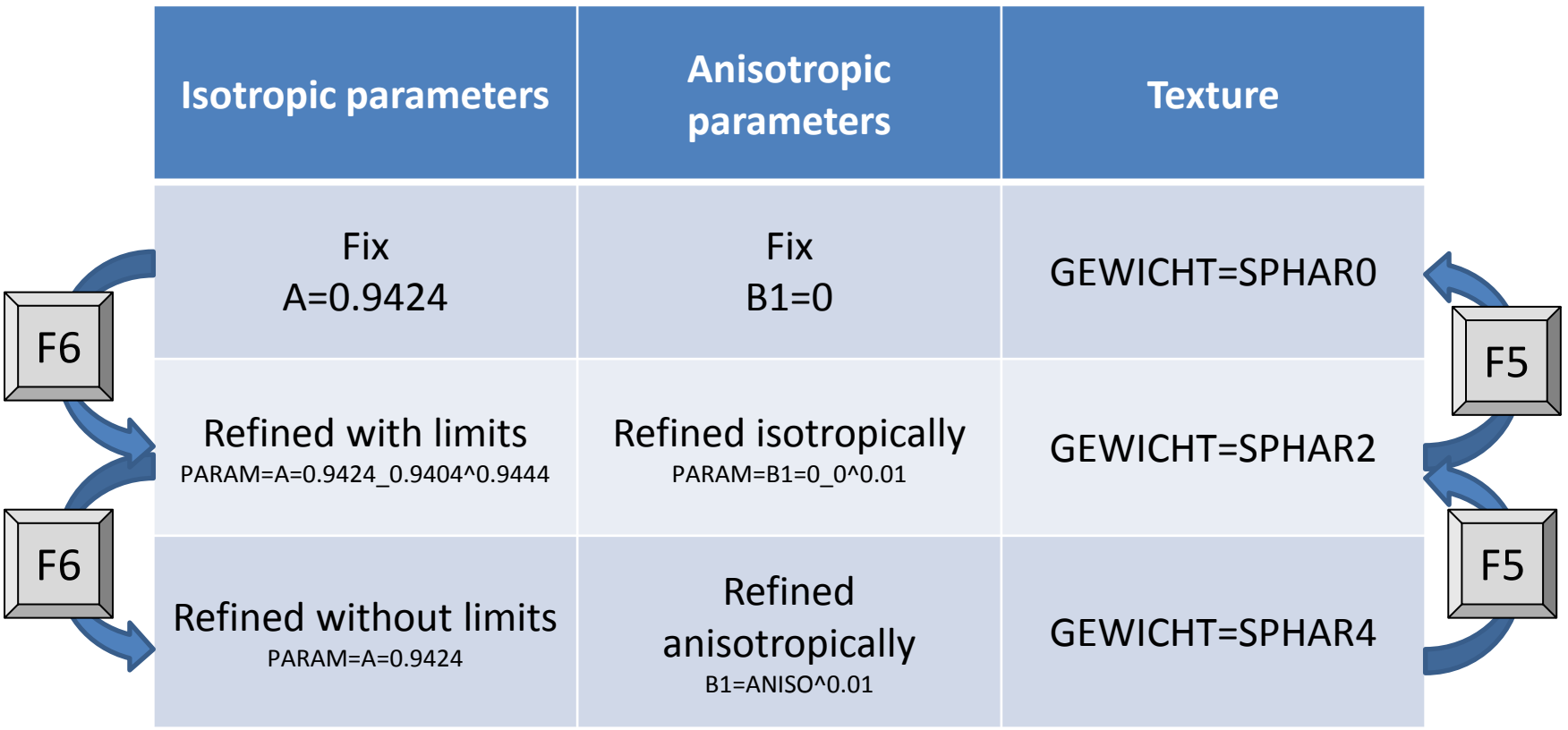
«refine isotropically»

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

F6: fix → isotropic → anisotropic

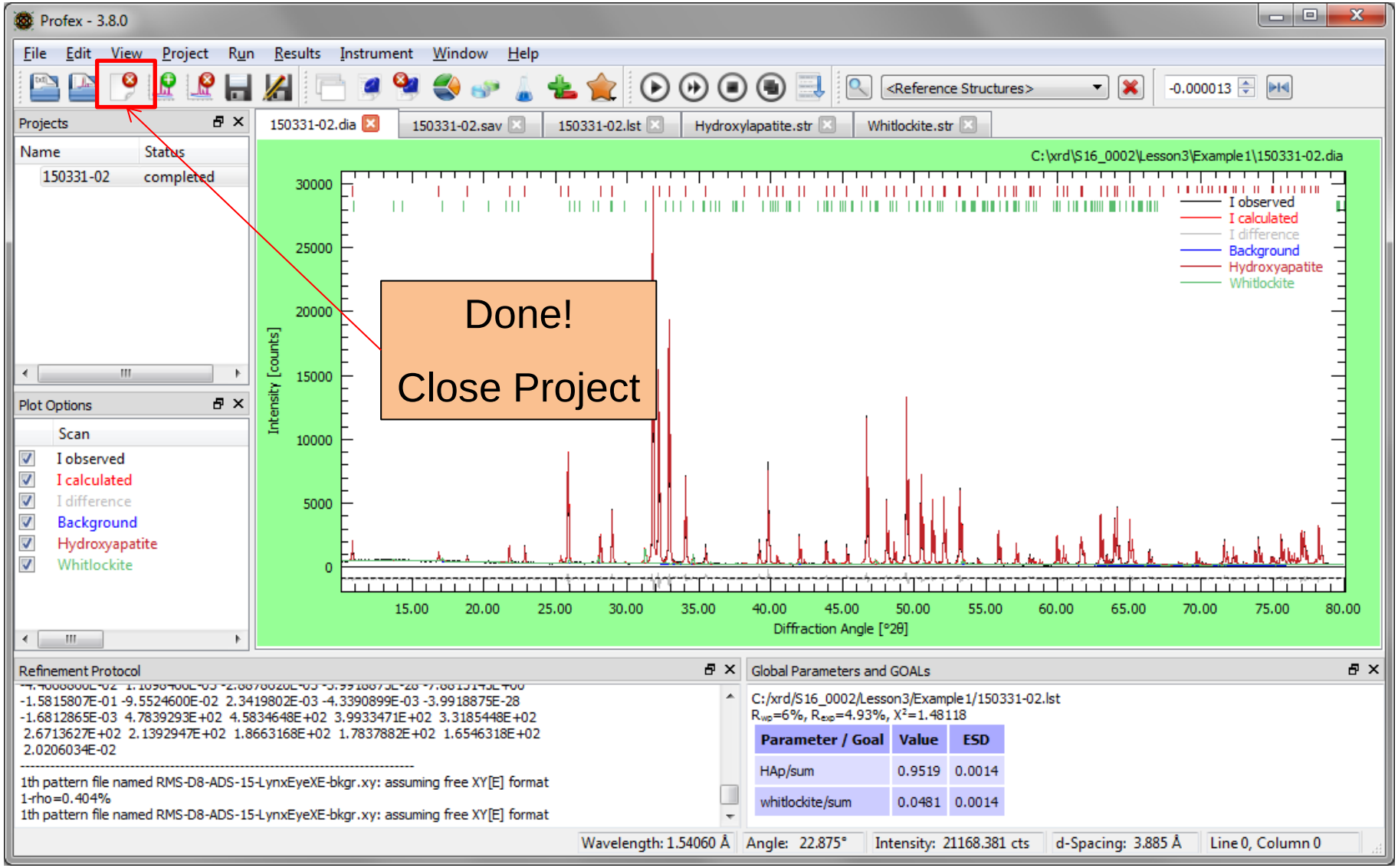
F5: anisotropic → isotropic → fix

Toggling Parameter Refinement States



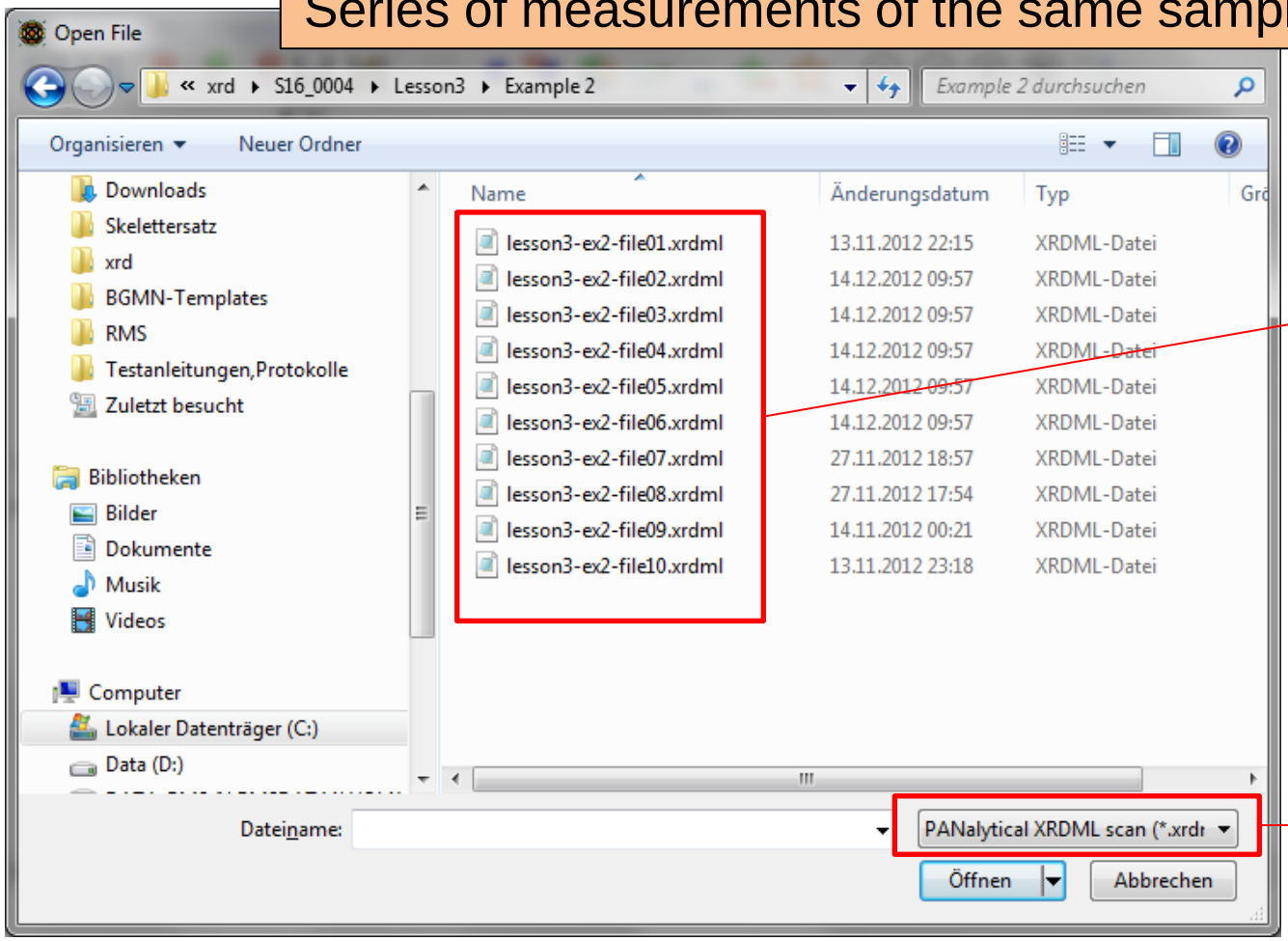
Isotropic parameters	Anisotropic parameters	Texture
Fix A=0.9424	Fix B1=0	GEWICHT=SPHAR0
Refined with limits PARAM=A=0.9424_0.9404^0.9444	Refined isotropically PARAM=B1=0_0^0.01	GEWICHT=SPHAR2
Refined without limits PARAM=A=0.9424	Refined anisotropically B1=ANISO^0.01	GEWICHT=SPHAR4

Optimized Refinement



Example 2: Batch Refinement

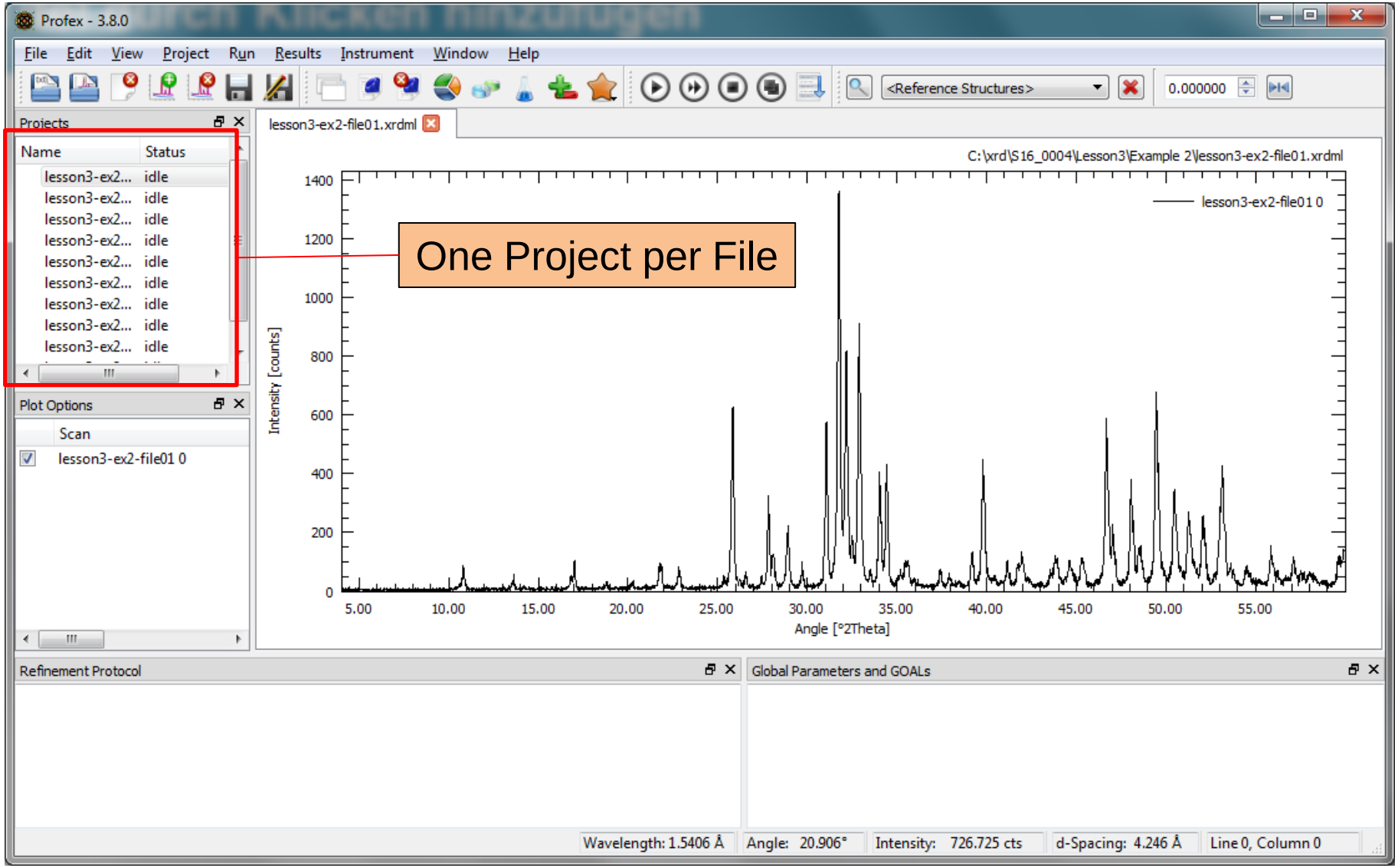
Series of measurements of the same sample



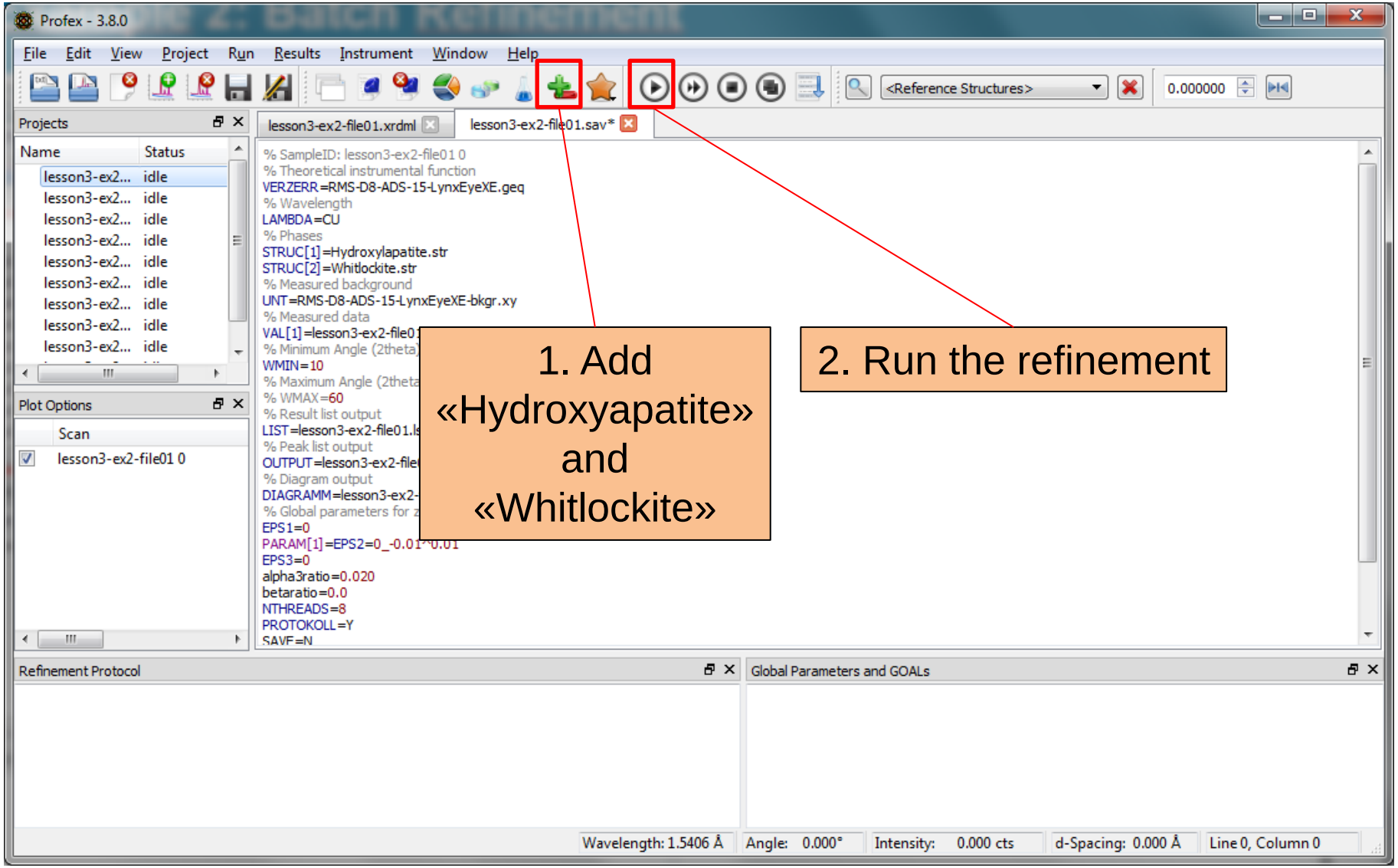
2. Select and open all files

1. Set Format

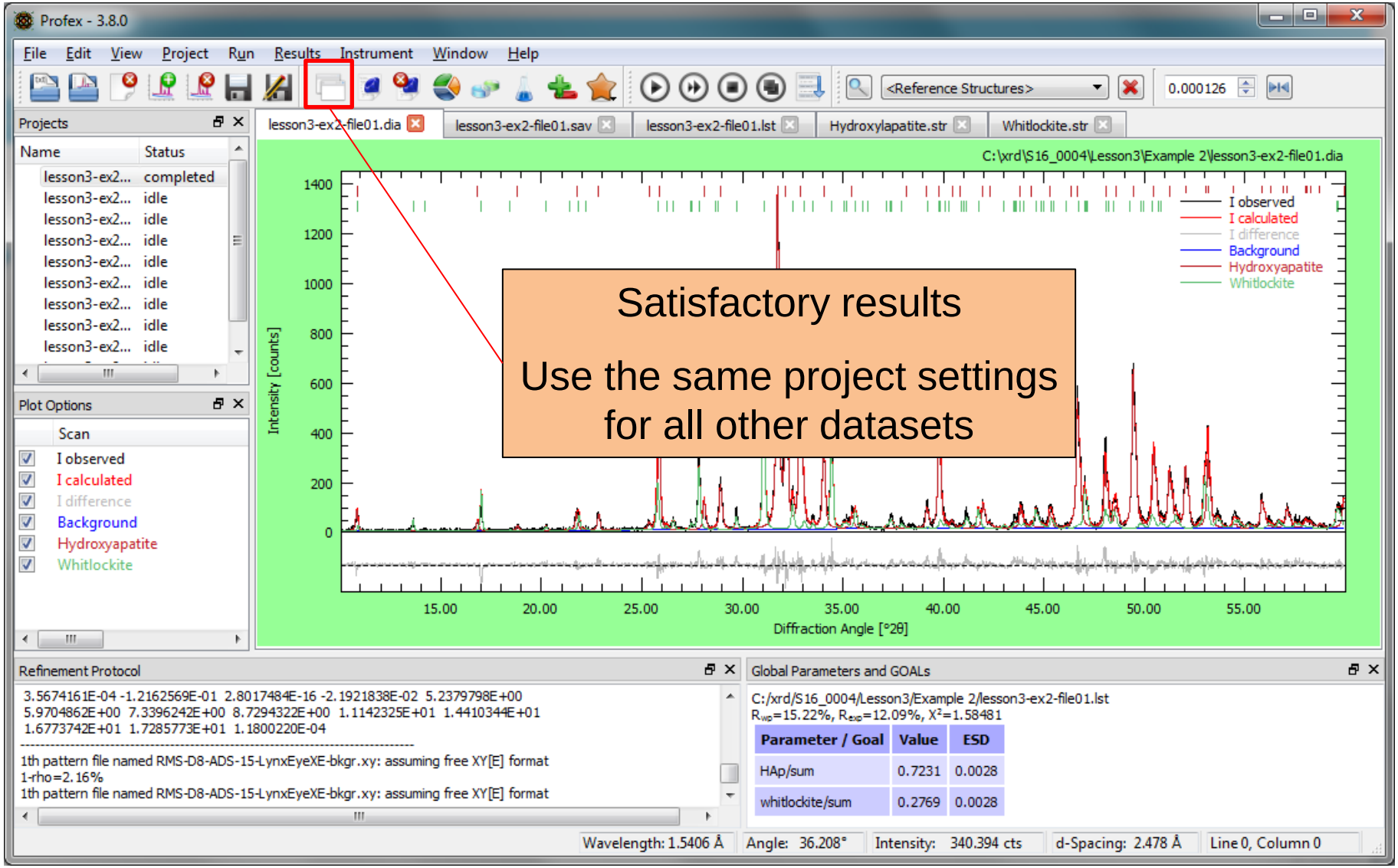
Example 2: Batch Refinement



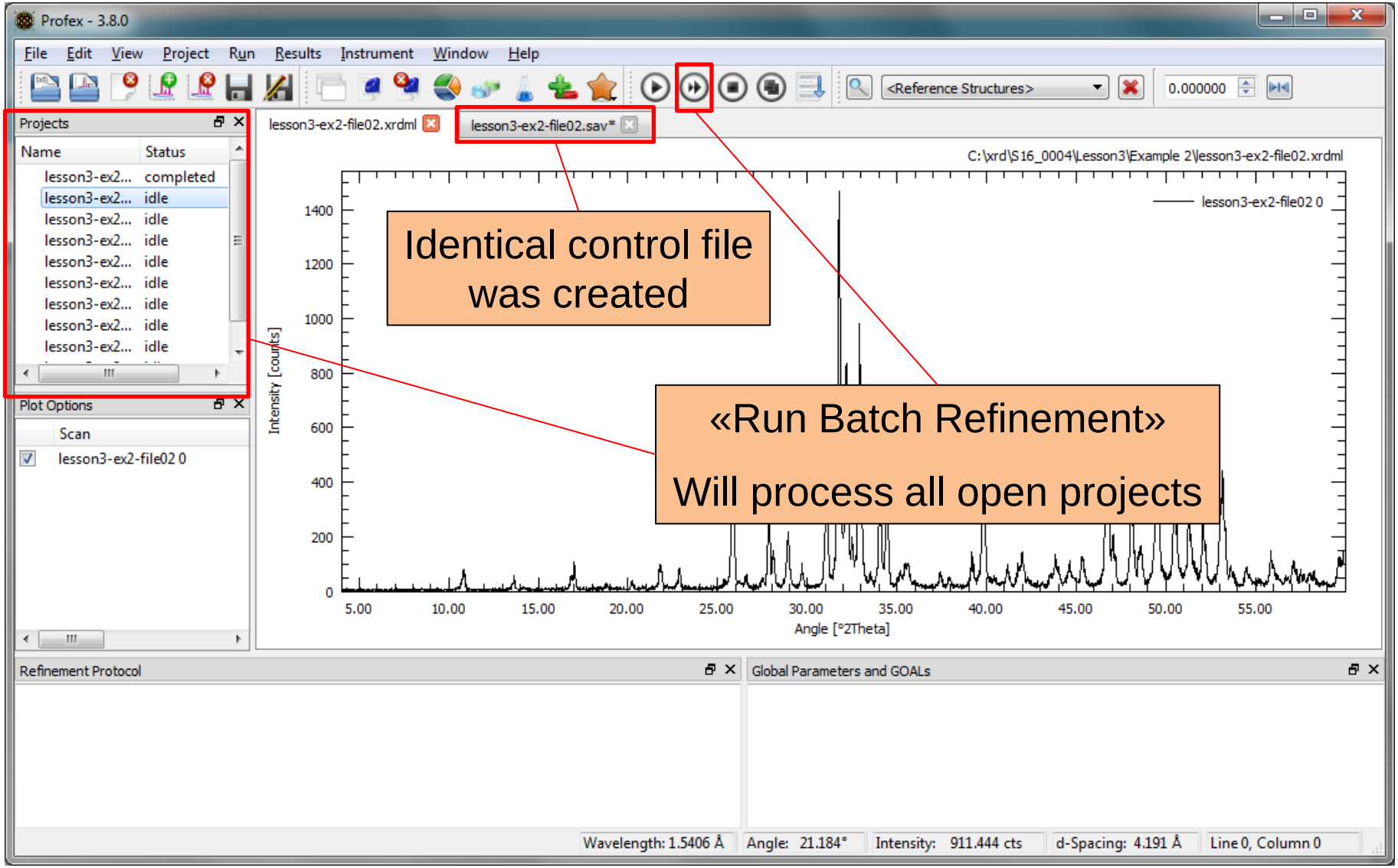
Example 2: Batch Refinement



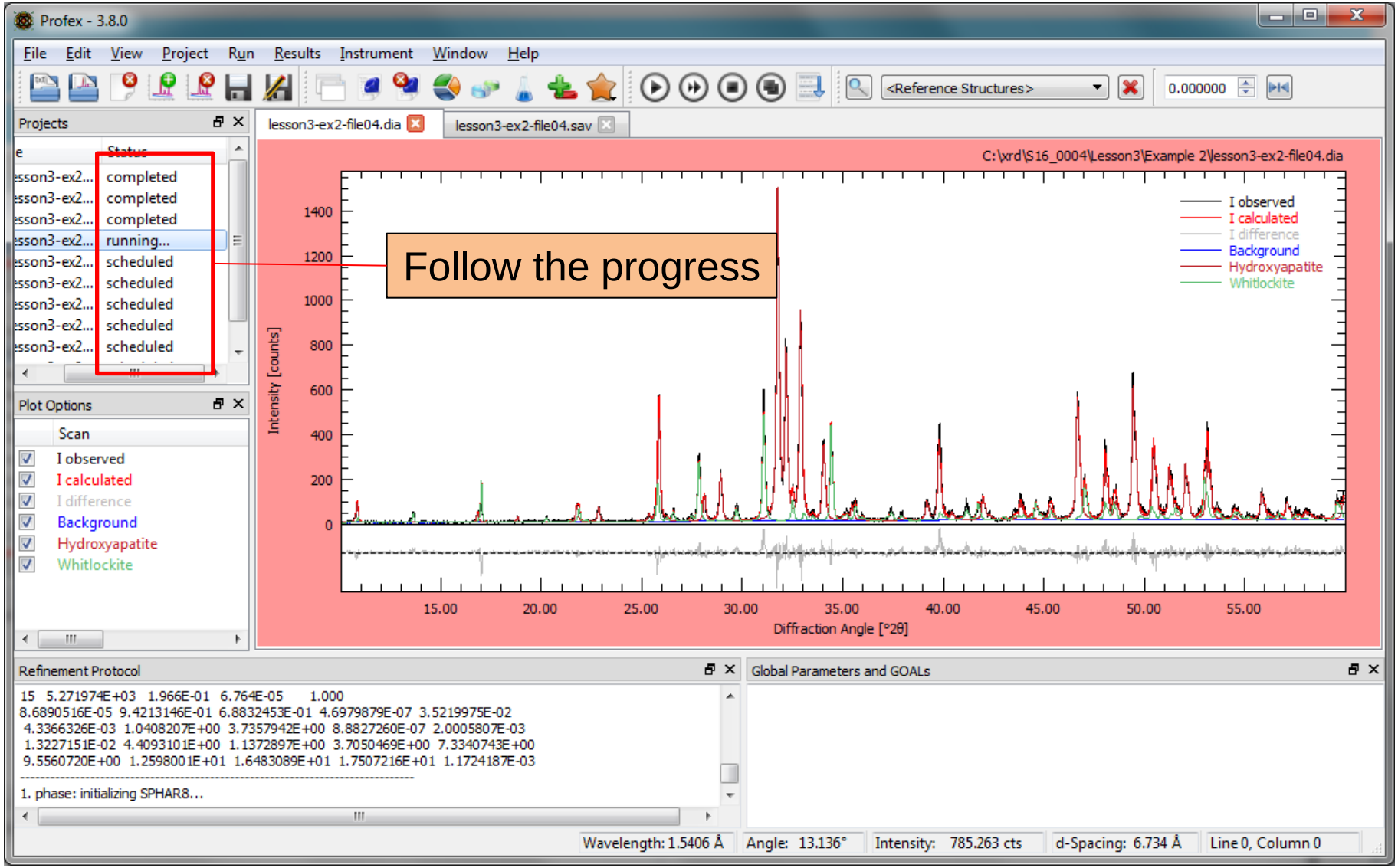
Example 2: Batch Refinement



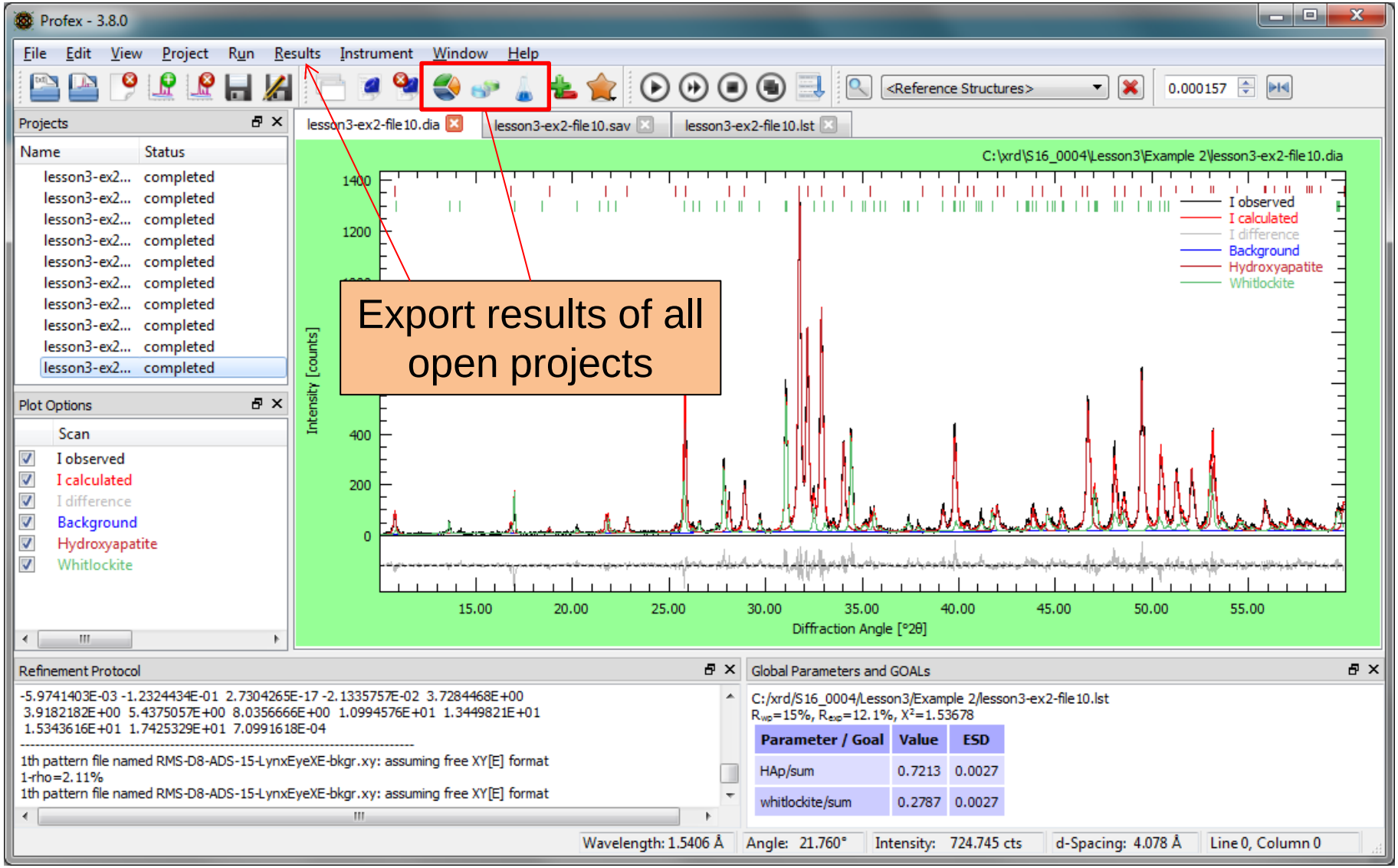
Example 2: Batch Refinement



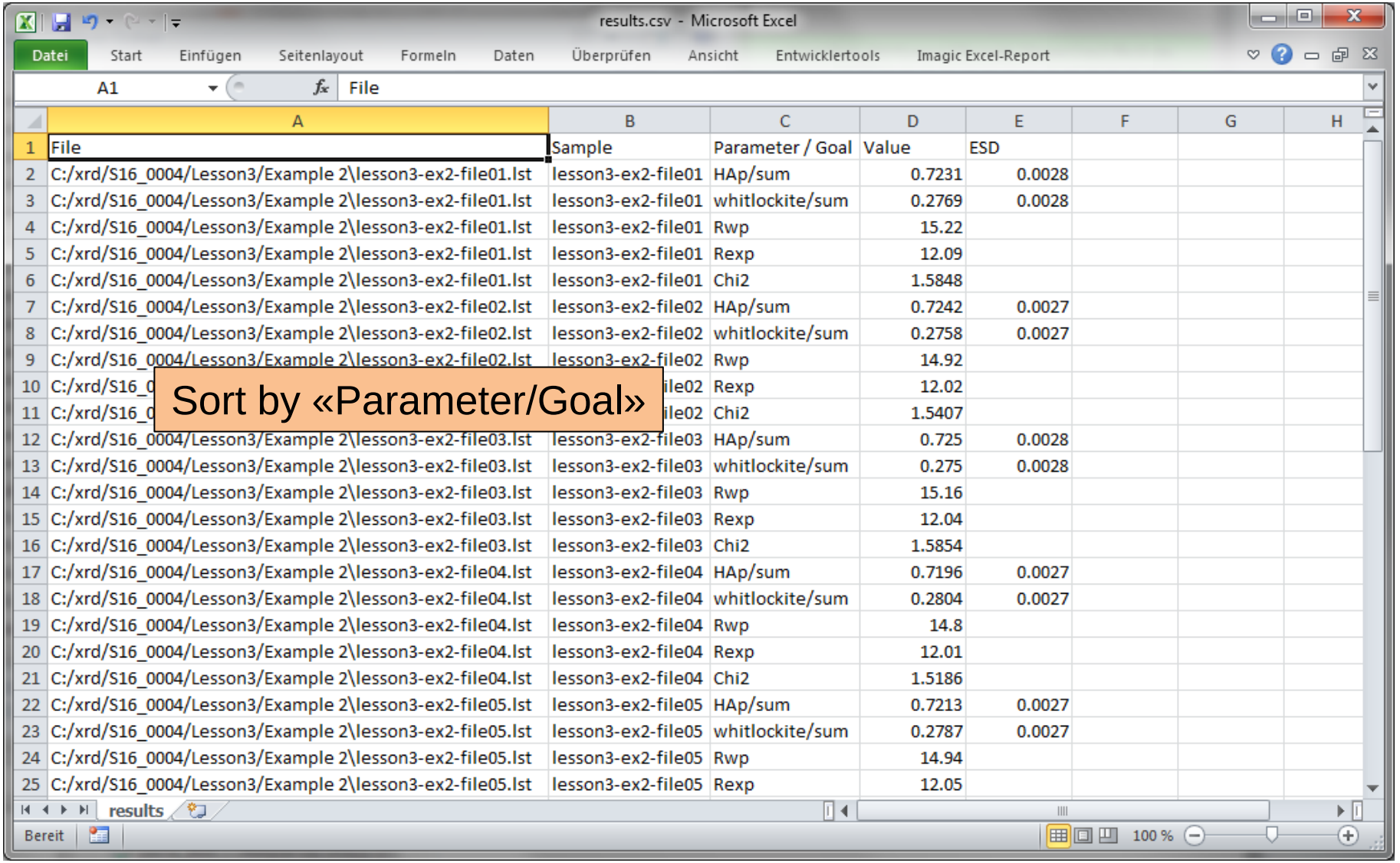
Example 2: Batch Refinement



Example 2: Batch Refinement

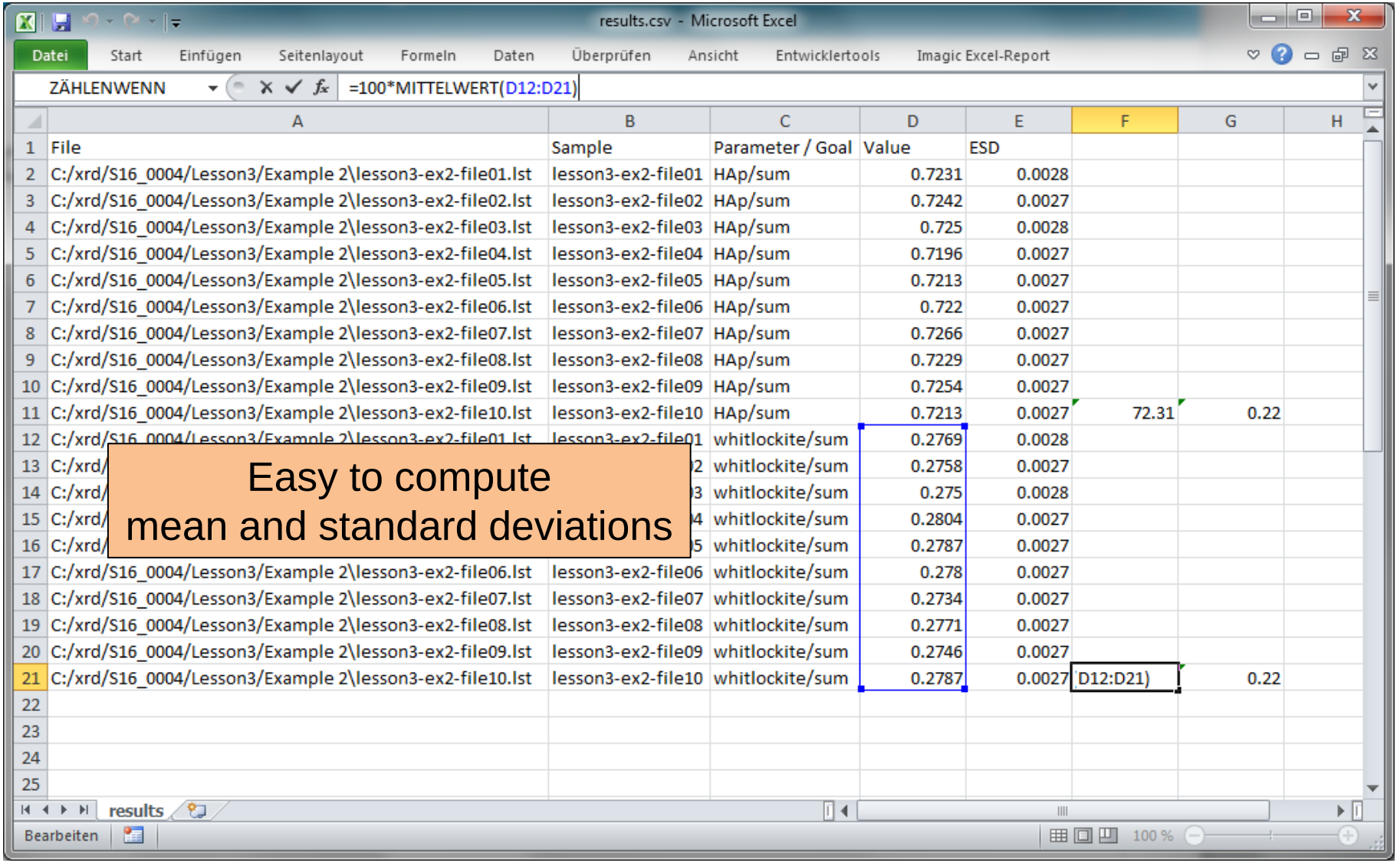


Exported Global GOALs



	A	B	C	D	E
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_0	ile02	Rexp	12.02	
11	C:/xrd/S16_0	ile02	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	

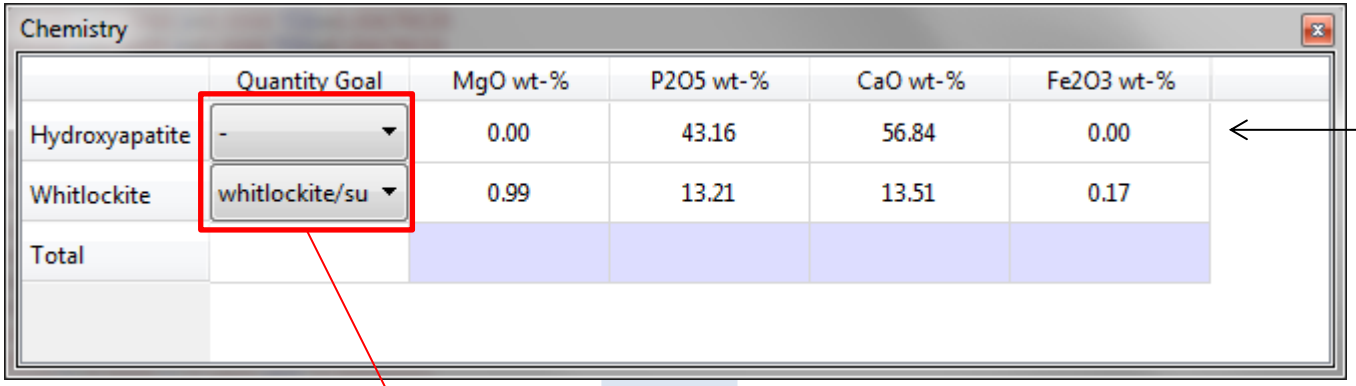
Exported Global GOALs



	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/	2	whitlockite/sum	0.2758	0.0027			
14	C:/xrd/	3	whitlockite/sum	0.275	0.0028			
15	C:/xrd/	4	whitlockite/sum	0.2804	0.0027			
16	C:/xrd/	5	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								

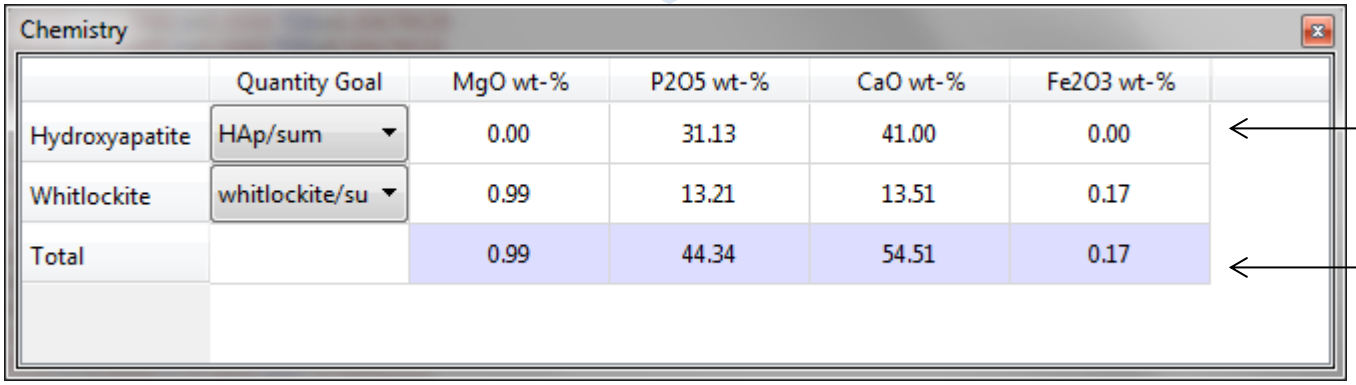
Refined Chemical Composition

Open «Window → Chemistry»



Normalized to 100%

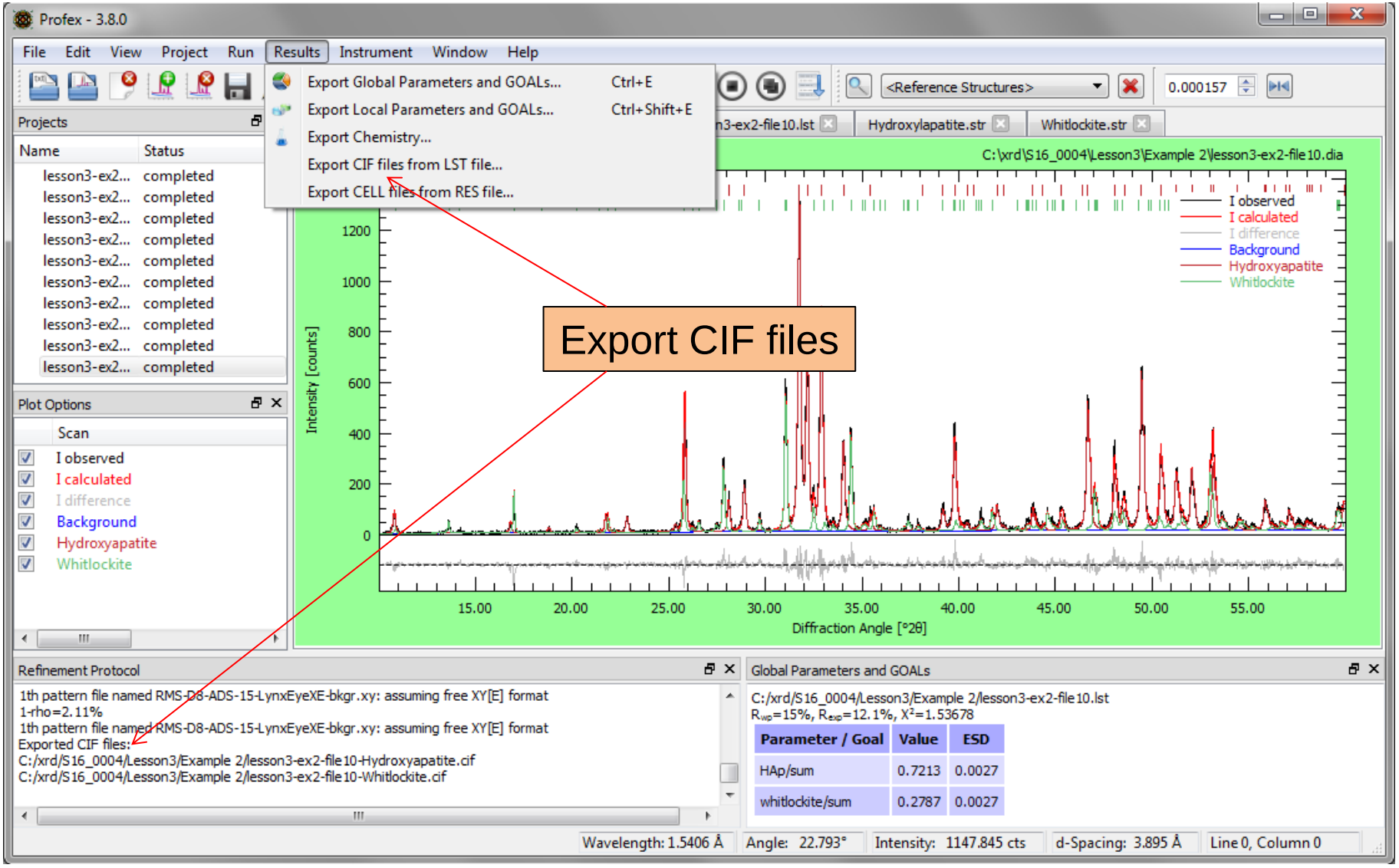
Make sure the Quantity GOALs are assigned correctly



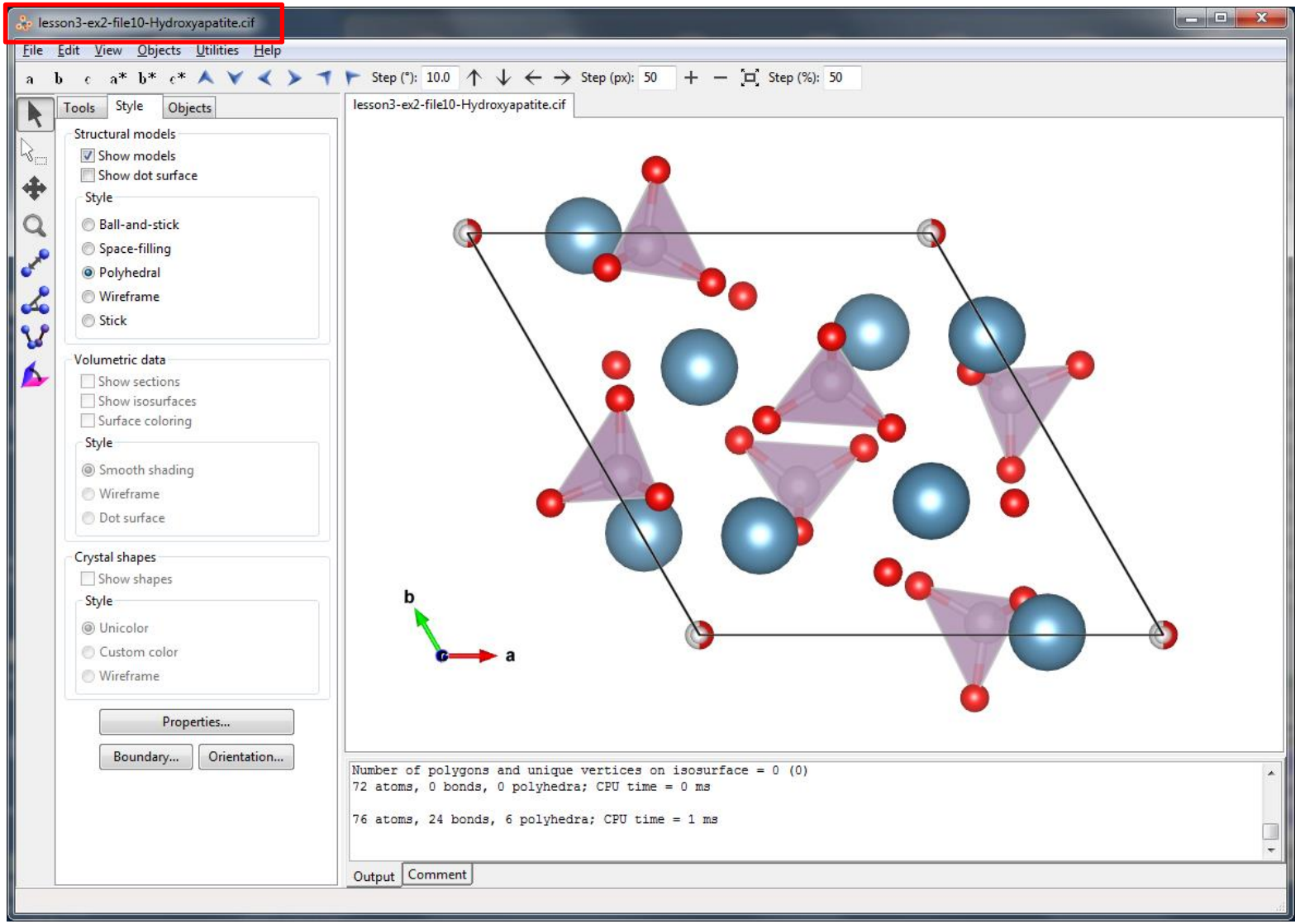
Normalized to refined phase quantity

Total sample composition available

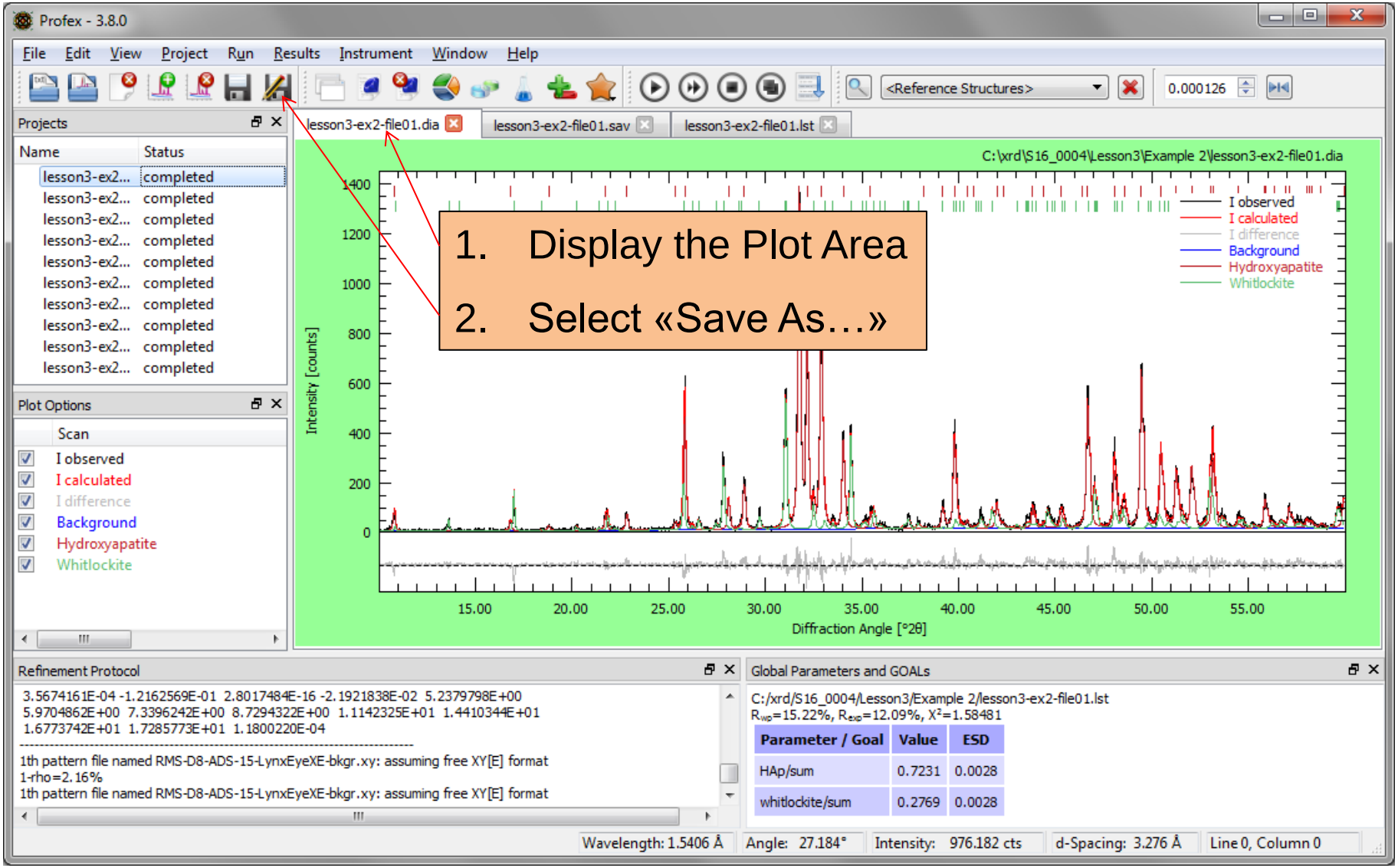
Create CIF files from refined structures



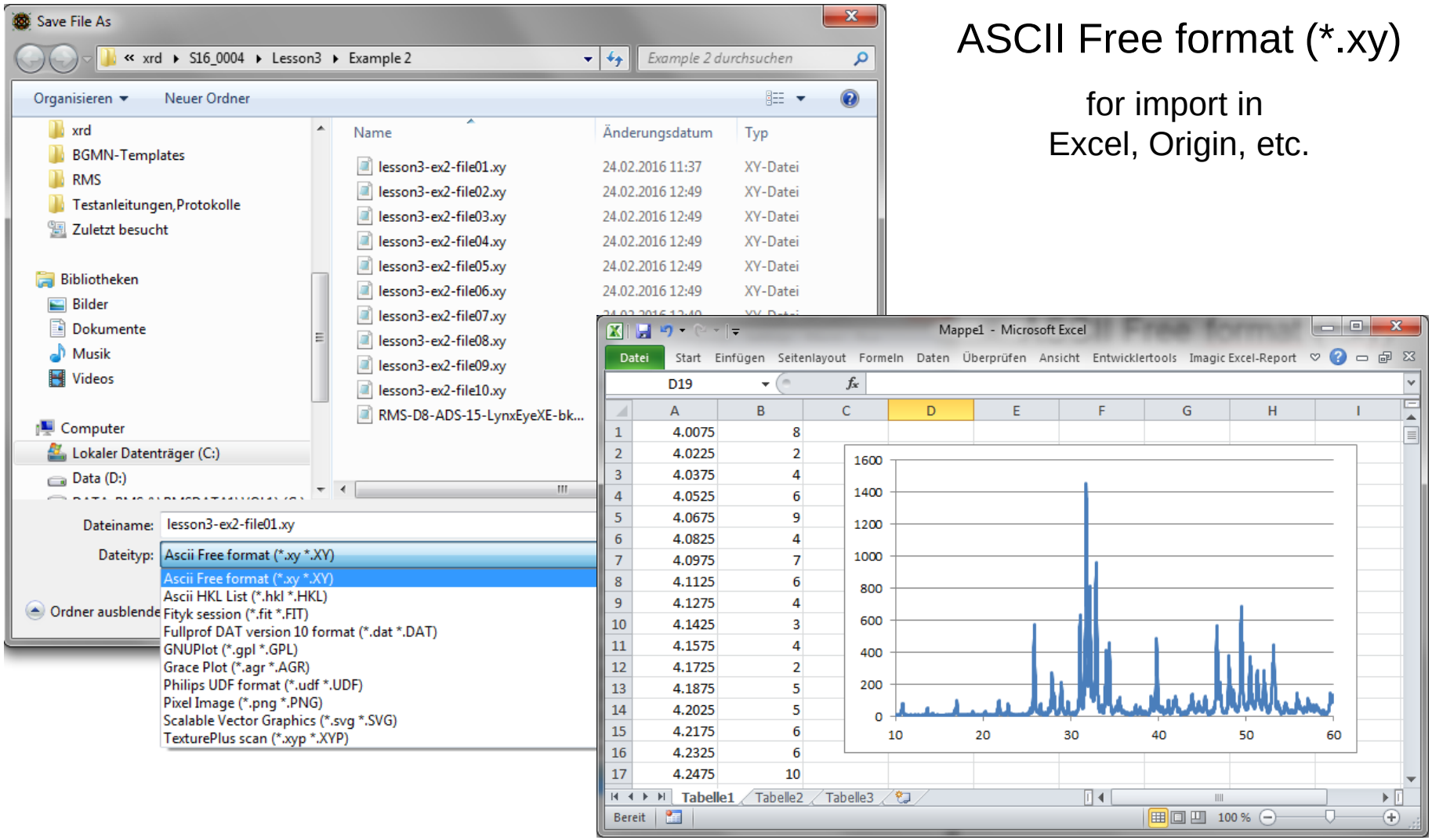
Drawing Structures



Exporting Diffraction Patterns



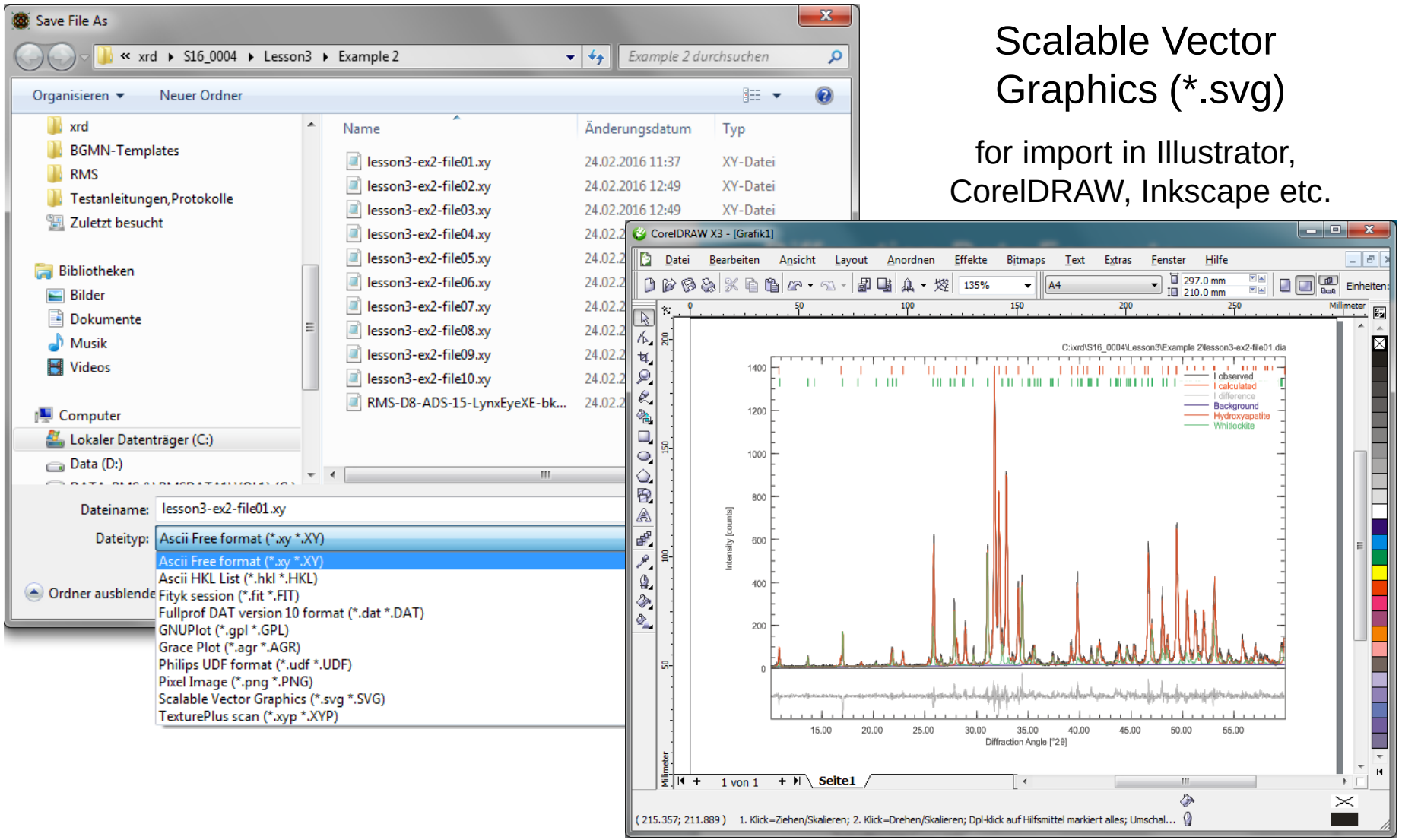
Diffraction Data Formats



ASCII Free format (*.xy)

for import in
Excel, Origin, etc.

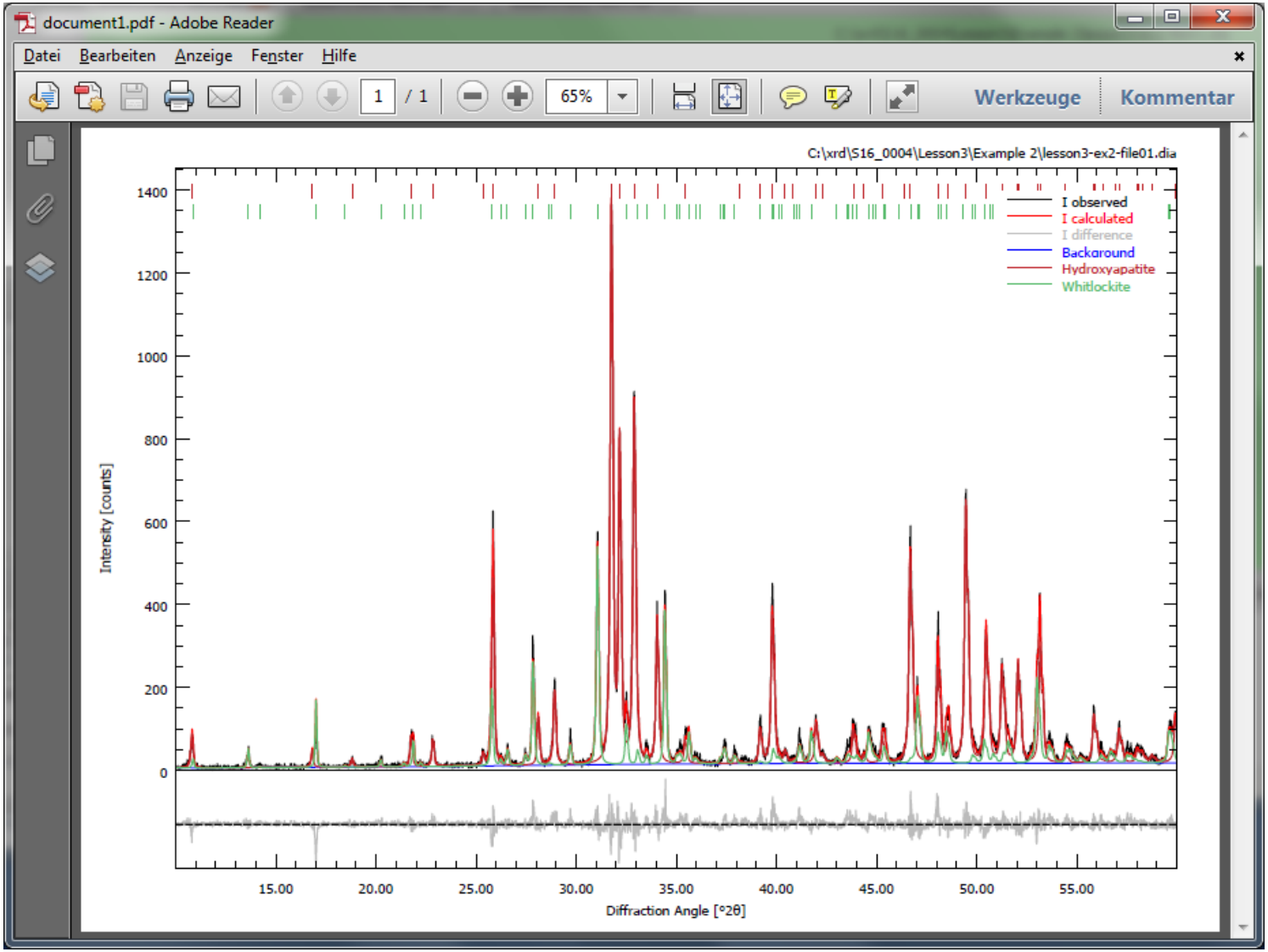
Diffraction Data Formats



Scalable Vector Graphics (*.svg)

for import in Illustrator, CorelDRAW, Inkscape etc.

Diffraction Data Formats



Profex

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

http://profex.doebelin.org