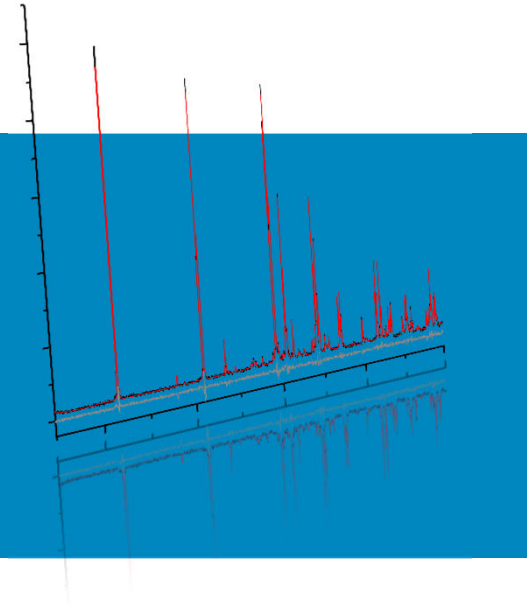
Lesson 6
BGMN & Profex



Nicola Döbelin
RMS Foundation, Bettlach, Switzerland

Rietveld Refinement Software BGMN

BGMN:

- Fundamental Parameters Approach
- Free for academic use
- Device independent
- Very robust automatic refinement strategy
- Slightly less steep learning curve
- Powerful scripting language
- Multi-Platform
- Multi-threaded

Visit: http://www.bgmn.de for tutorials and documentation

BGMN Website

Program Description

Site map

Up | Program Description | BGMN FAQ | Download Page

- Instrumental Function
- Tube Tails and size/strain estimation
- Structure Description
- Download Structures
- Preferred Orientation
- Calculation Control
- Result Output
- BGMN Variables

The following pages serve as a short introduction into the BGMN Rietveld software. A description of an example (plaster) makes your test runs easier.

First, the generation of the instrumental function is described.

Second, the construction of structure files is explained. In an extra topic the handling of preferred orientation is mentioned in detail.

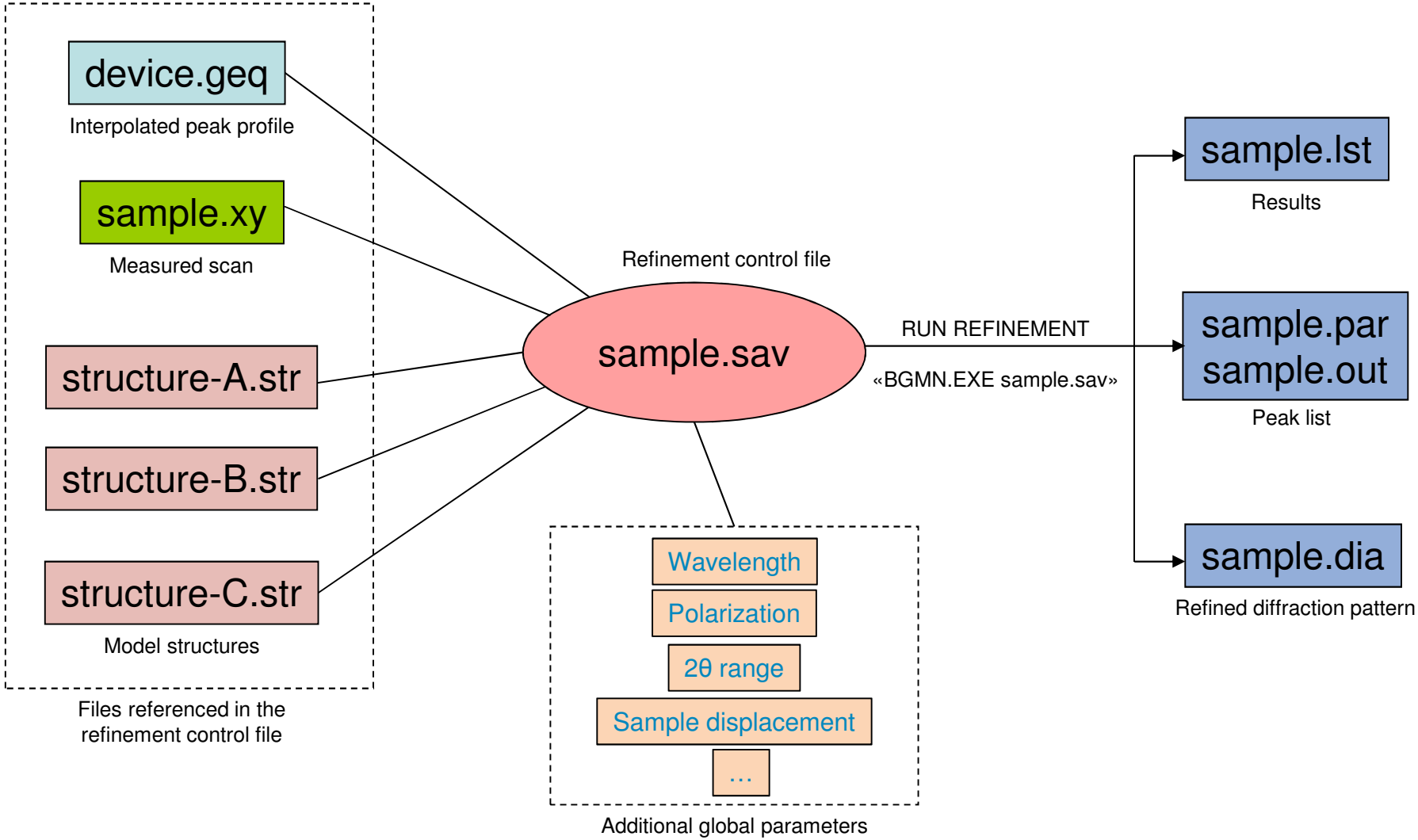
Third, the calculation control during a problem specific control file is shown.

Last, we have a look at the different result files.

A somewhat extended explanation of the used variables is also available.

http://www.bgmn.de/program.html

BGMN Control File (*.sav)



Profex

Graphical User Interface (GUI) for BGMN

Developer:	Nicola Döbelin (private)
License:	GPL (open source)
Platforms:	Windows XP / Vista / 7 / 8 Linux Mac OS X 10.6.8-10.9.2 (64bit)
Rietveld Backends:	BGMN, Fullprof.2k
Website:	http://profex.doebelin.org
Current stable version:	3.3.1

History

2003: Start of development as an alternative GUI for Fullprof.2k

For personal use only (my PhD)

Linux only

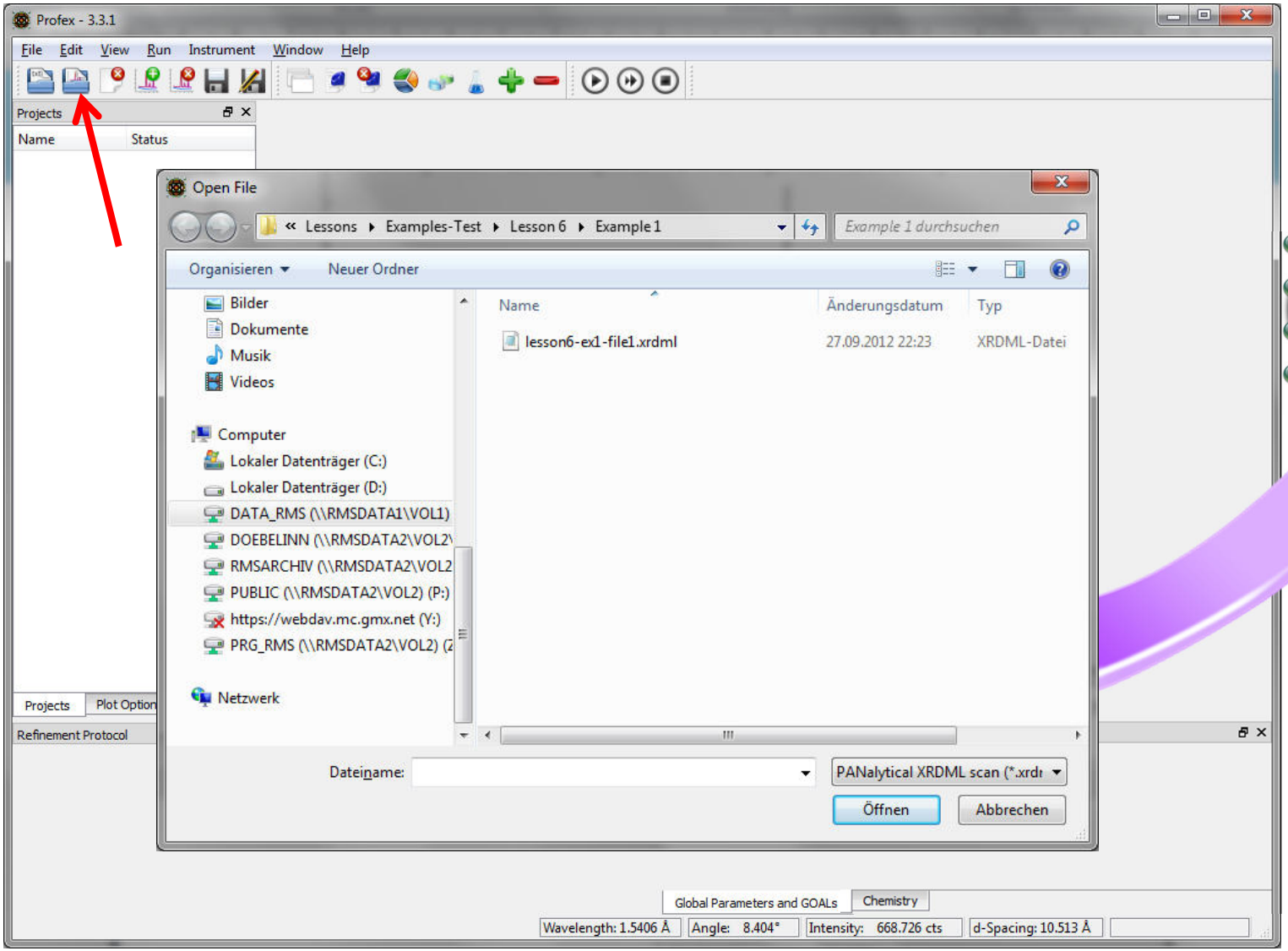
2006: Major rewrite

Support for Windows

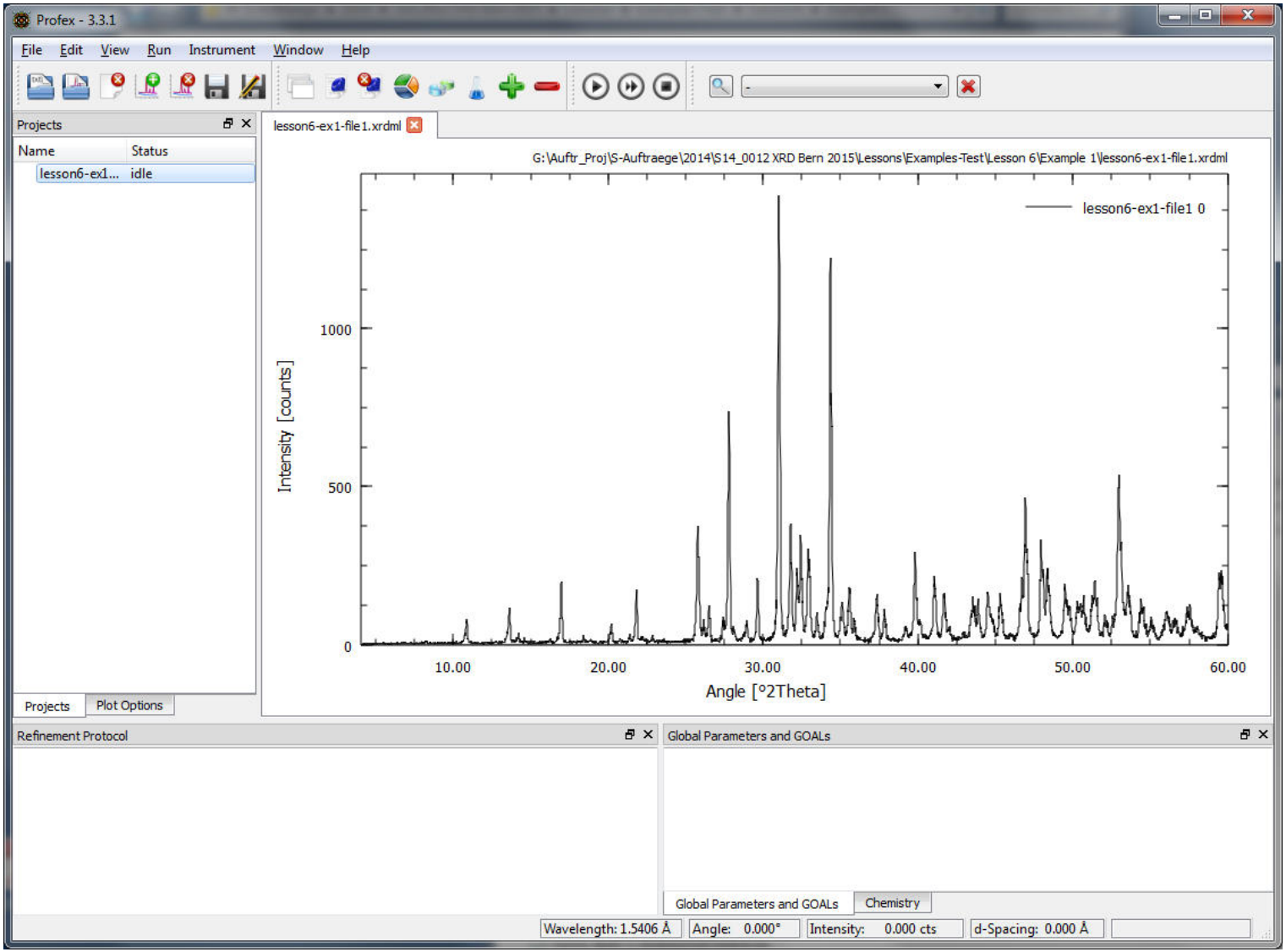
2012: Support for BGMN Rietveld backend added

2014: Support for Mac OS X

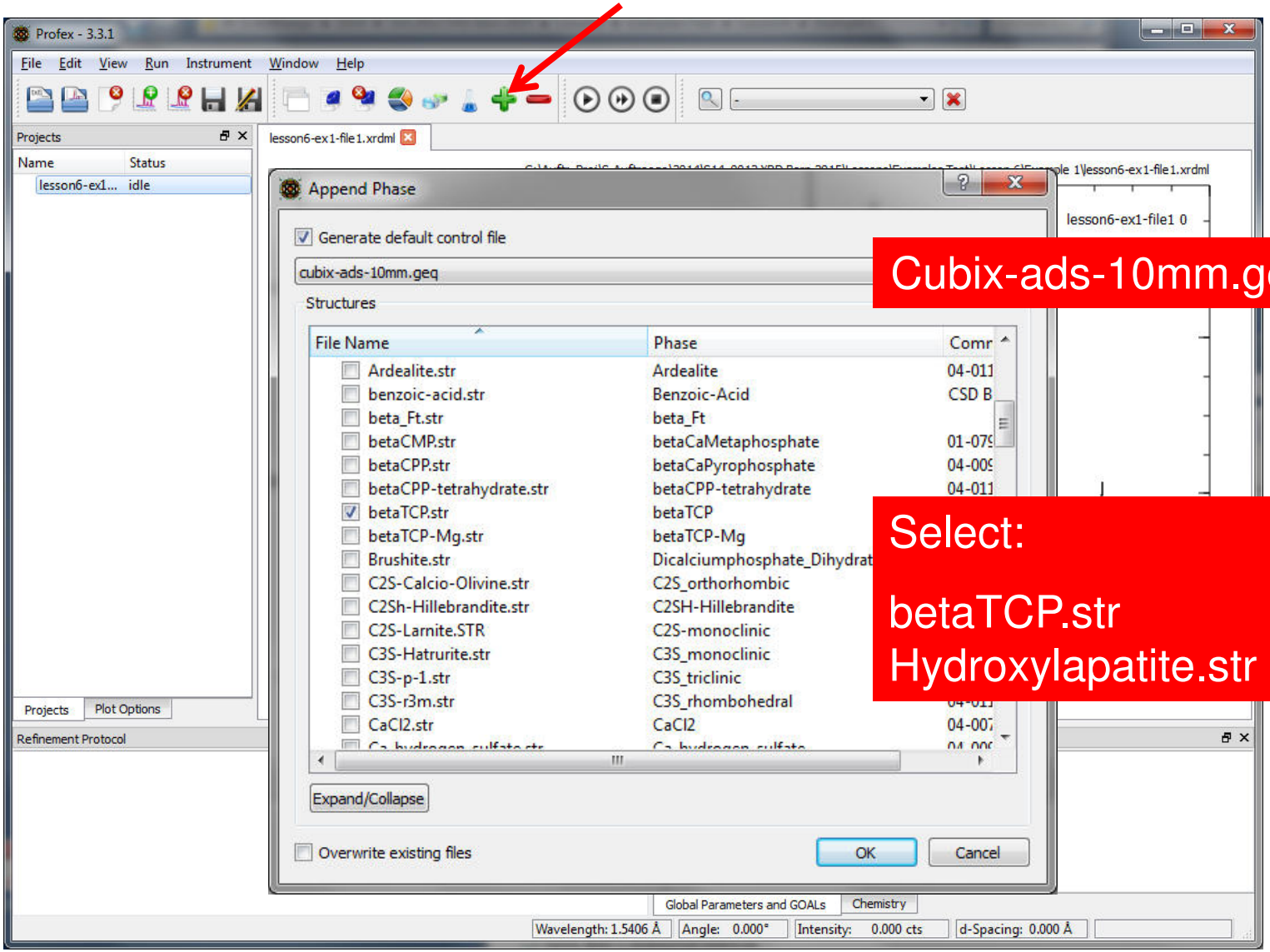
First Use


Profex - 3.3.1
File Edit View Run Instrument Window Help
Projects
Name Status
Open File
« Lessons ▸ Examples-Test ▸ Lesson 6 ▸ Example 1
Example 1 durchsuchen
Organisieren Neuer Ordner
Bilder
Dokumente
Musik
Videos
Computer
Lokaler Datenträger (C:)
Lokaler Datenträger (D:)
DATA_RMS (\\RMSDATA1\VOL1)
DOEBELINN (\\RMSDATA2\VOL2\
RMSARCHIV (\\RMSDATA2\VOL2
PUBLIC (\\RMSDATA2\VOL2) (P:)
https://webdav.mc.gmx.net (Y:)
PRG_RMS (\\RMSDATA2\VOL2) (
Netzwerk
Name
Änderungsdatum
Typ
lesson6-ex1-file1.xrdml
27.09.2012 22:23
XRDML-Datei
Dateiname:
PANalytical XRDML scan (*.xrd
Öffnen
Abbrechen
Projects
Plot Option
Refinement Protocol
Global Parameters and GOALs
Chemistry
Wavelength: 1.5406 Å
Angle: 8.404°
Intensity: 668.726 cts
d-Spacing: 10.513 Å
Profex

Lesson 6: Example 1



Lesson 6: Example 1

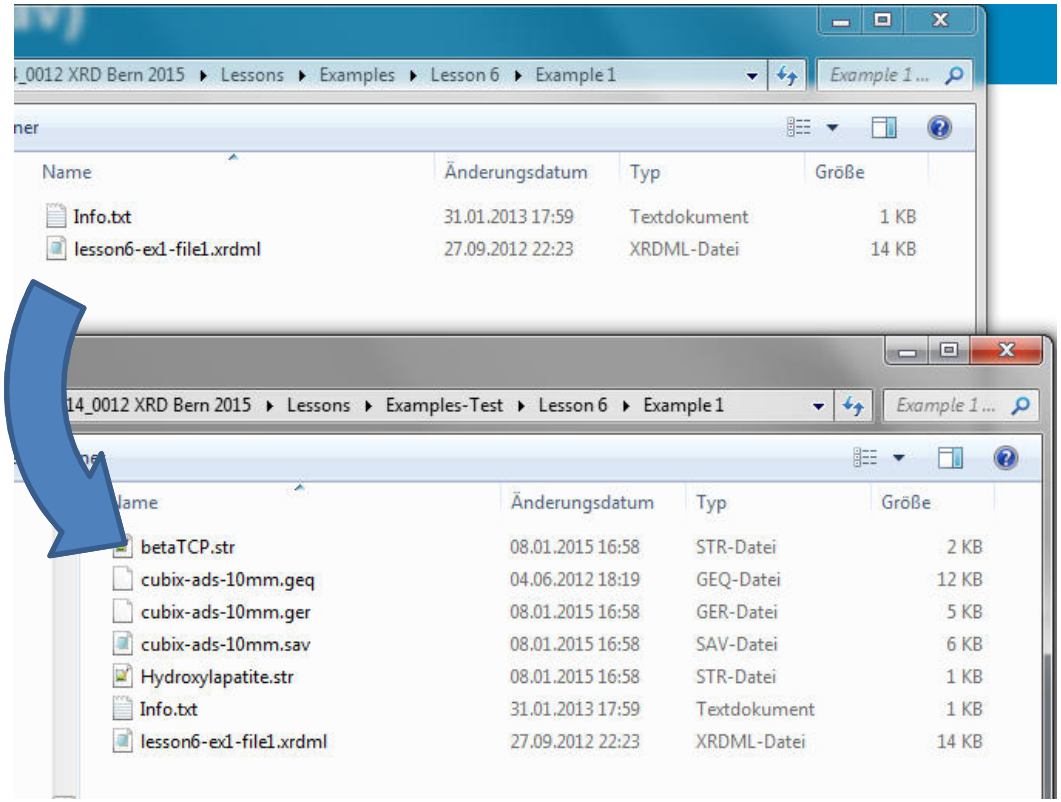


Lesson 6: Example 1

BGMN Control File (*.sav)

What Profex does in the background:

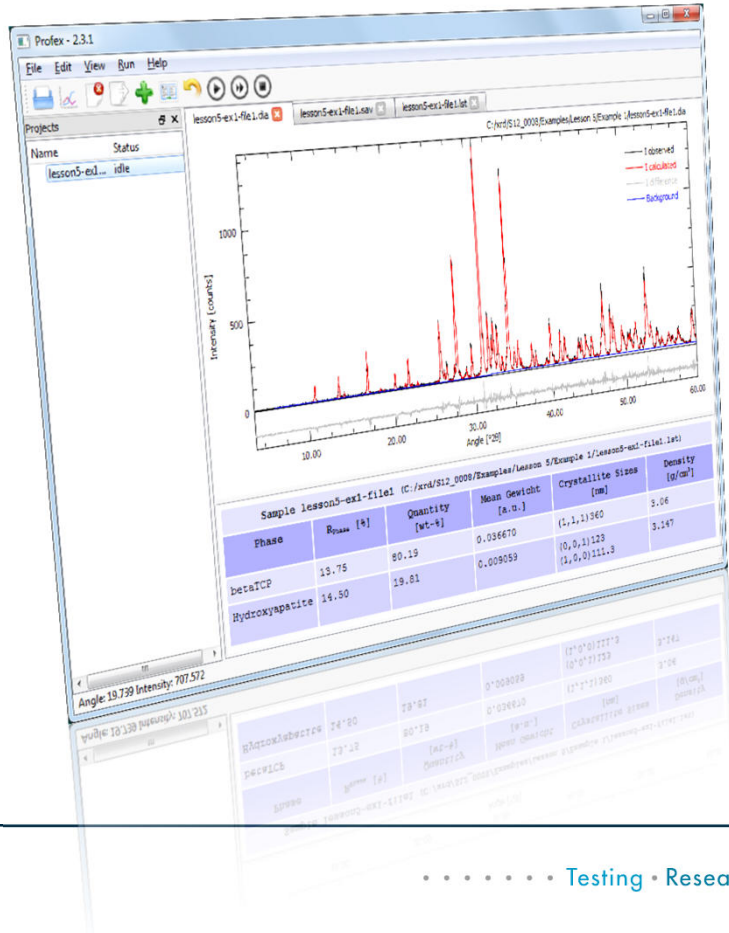
- Generate a control file
- Adjust file names in control file
- Copy all selected **structure files** from local DB to location of scan file
- Copy **instrument configuration files** from local DB to location of the scan file



Profex

With Profex:

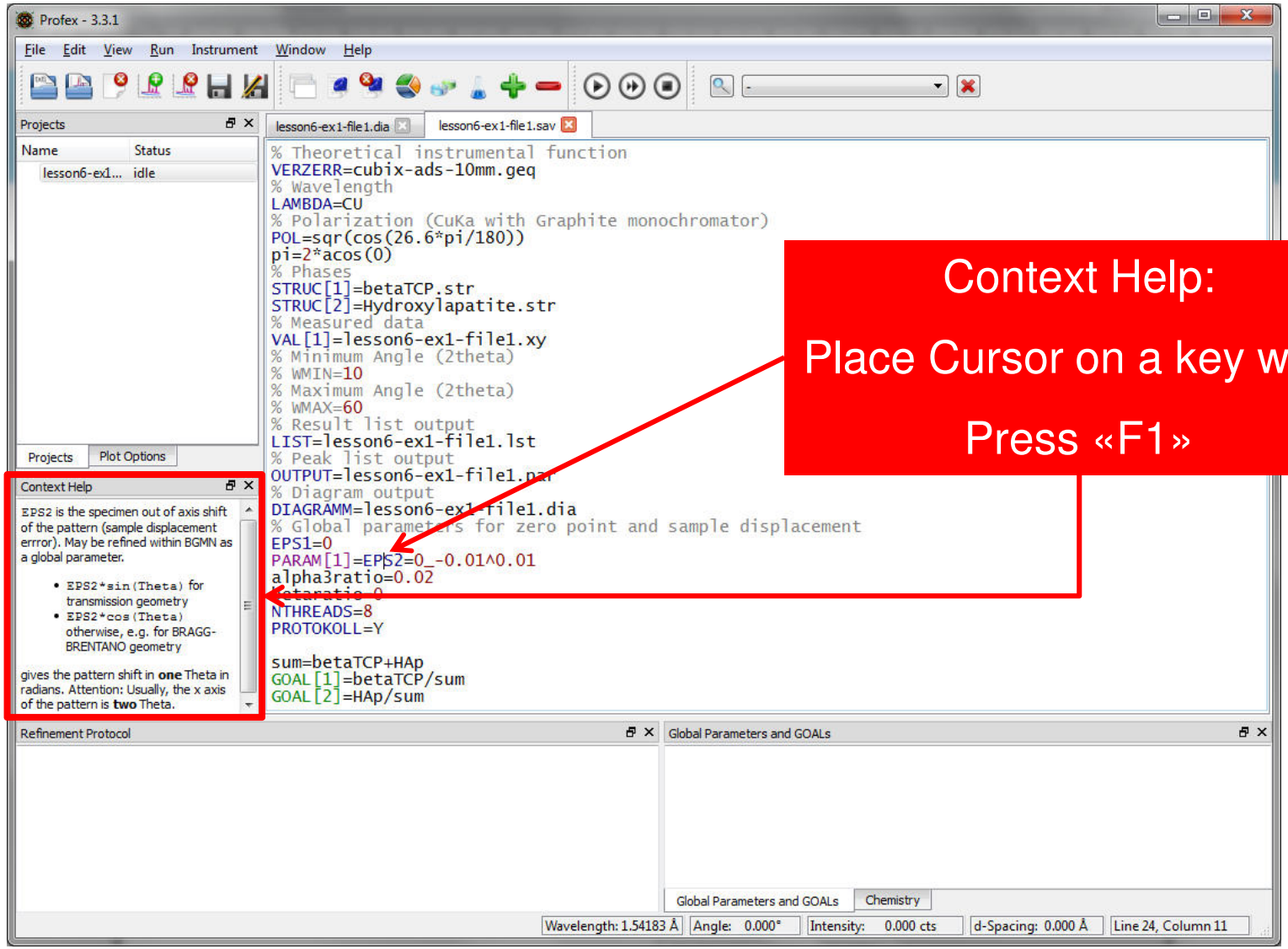
1. Load scan file
2. Use «Add phase» dialog to select phases, instrument, and generate control file
3. Run refinement



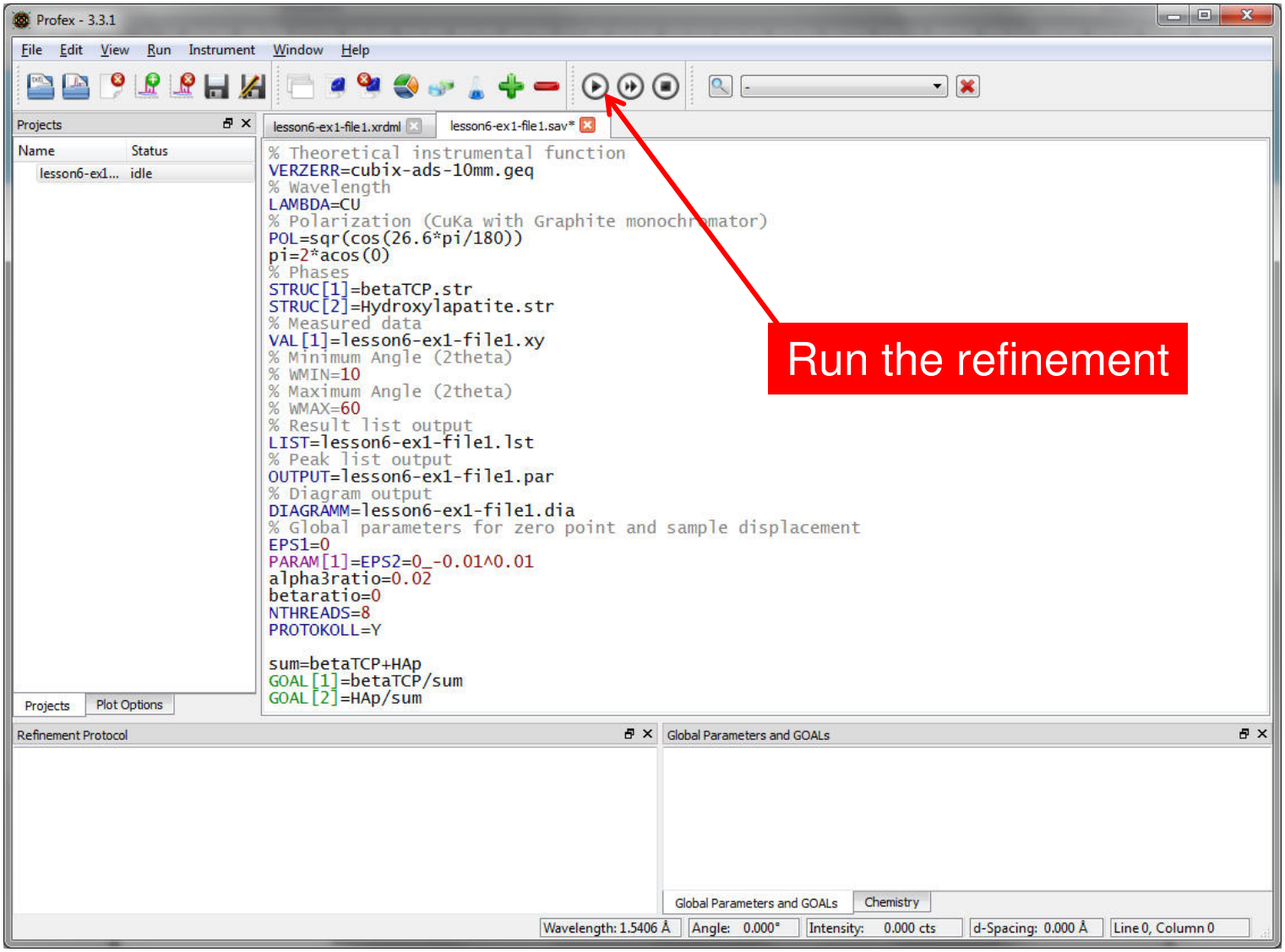
No need to:

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

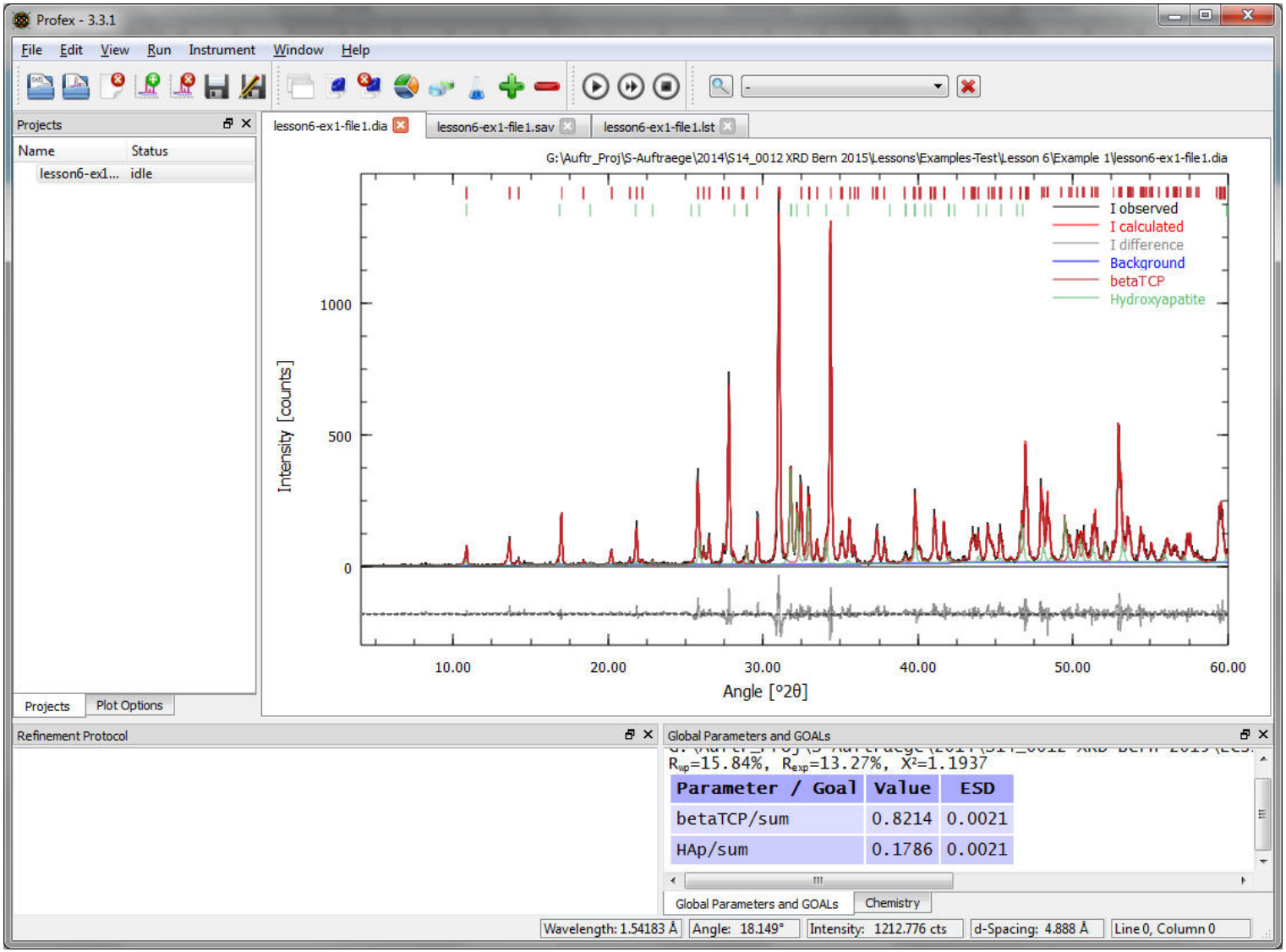
Lesson 6: Example 1



Lesson 6: Example 1



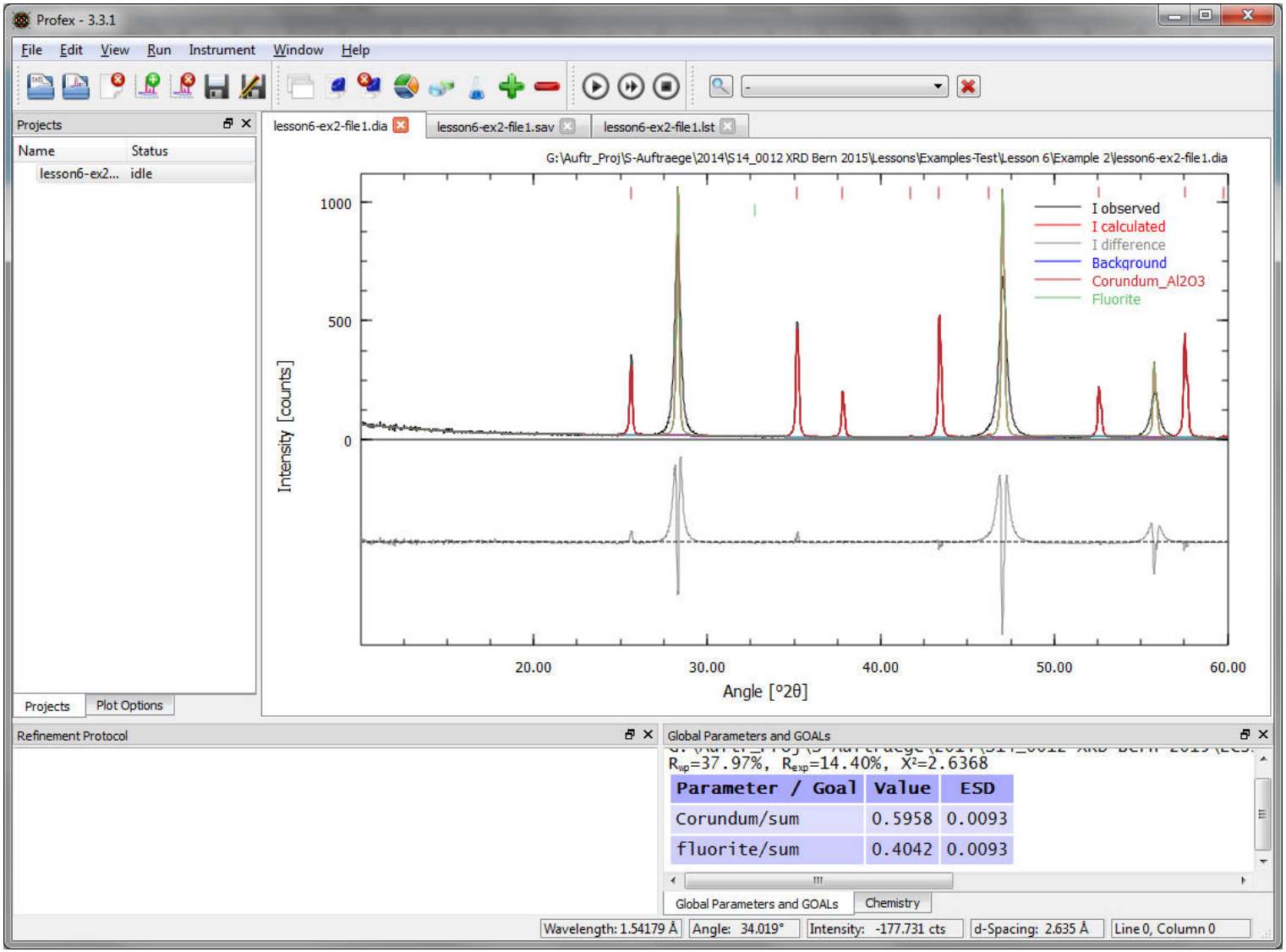
Lesson 6: Example 1



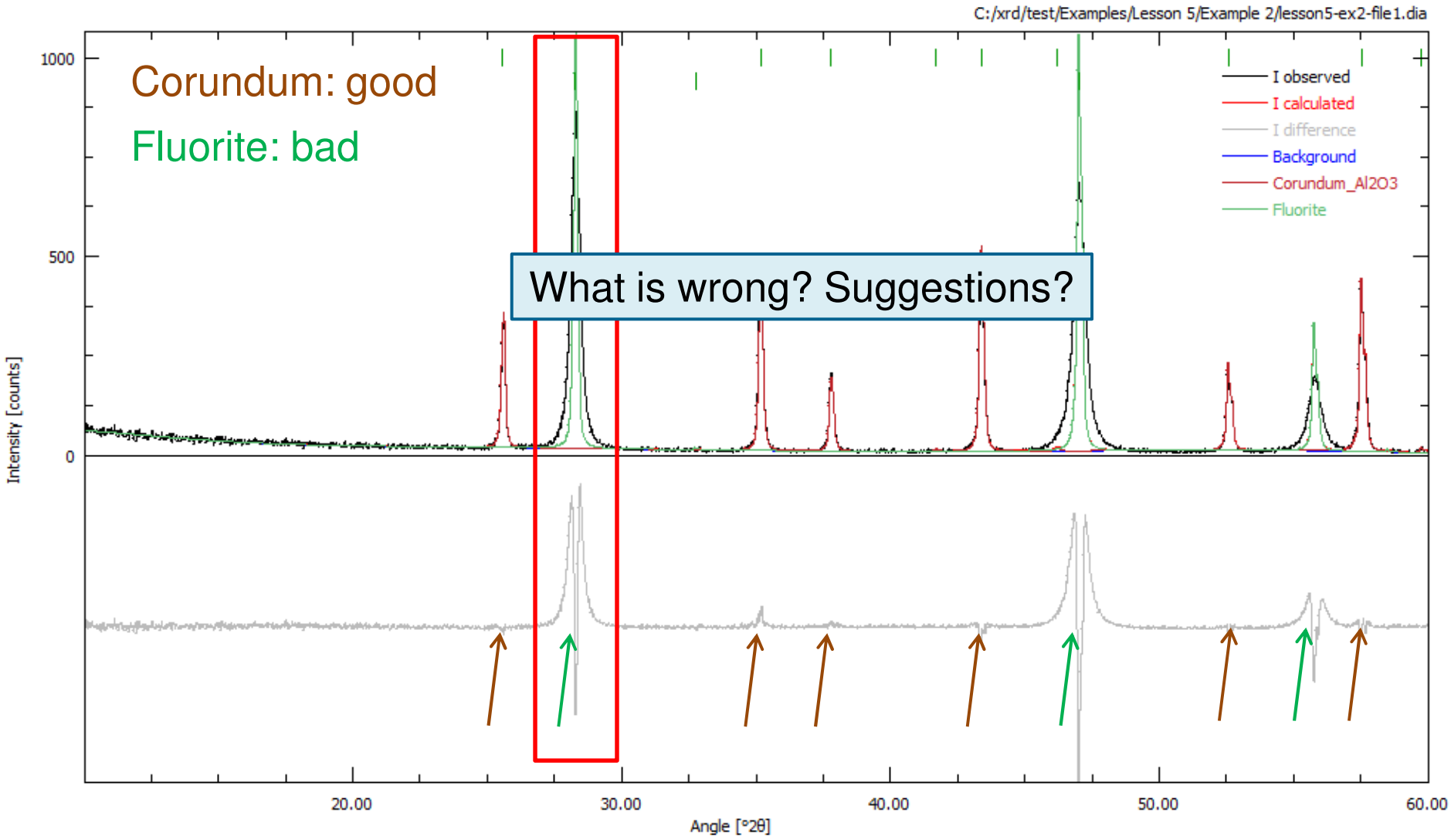
Lesson 6: Example 2

1. Open Graph File:
   «Examples\Lesson 6\Example 2\lesson6-ex2.file1.xrdml»
2. Click «Add a phase» (+)
   a) Select instrument: «pw1800-fds»
   b) Select Phases:
      «AL2O3-Corundum»
      «Fluorite»
3. Run the refinement

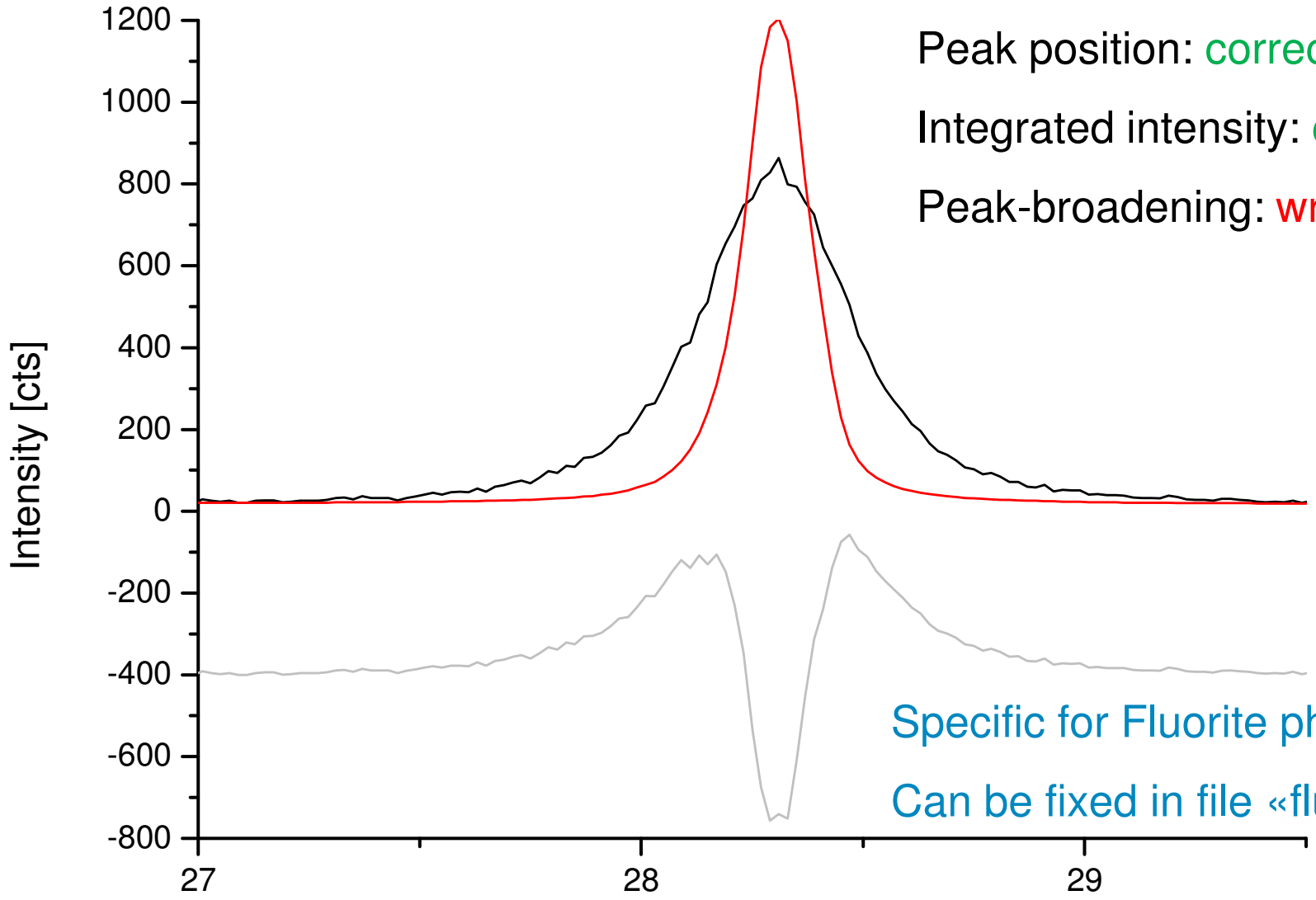
Lesson 6: Example 2



Lesson 6: Example 2



Lesson 6: Example 2



Peak position: correct

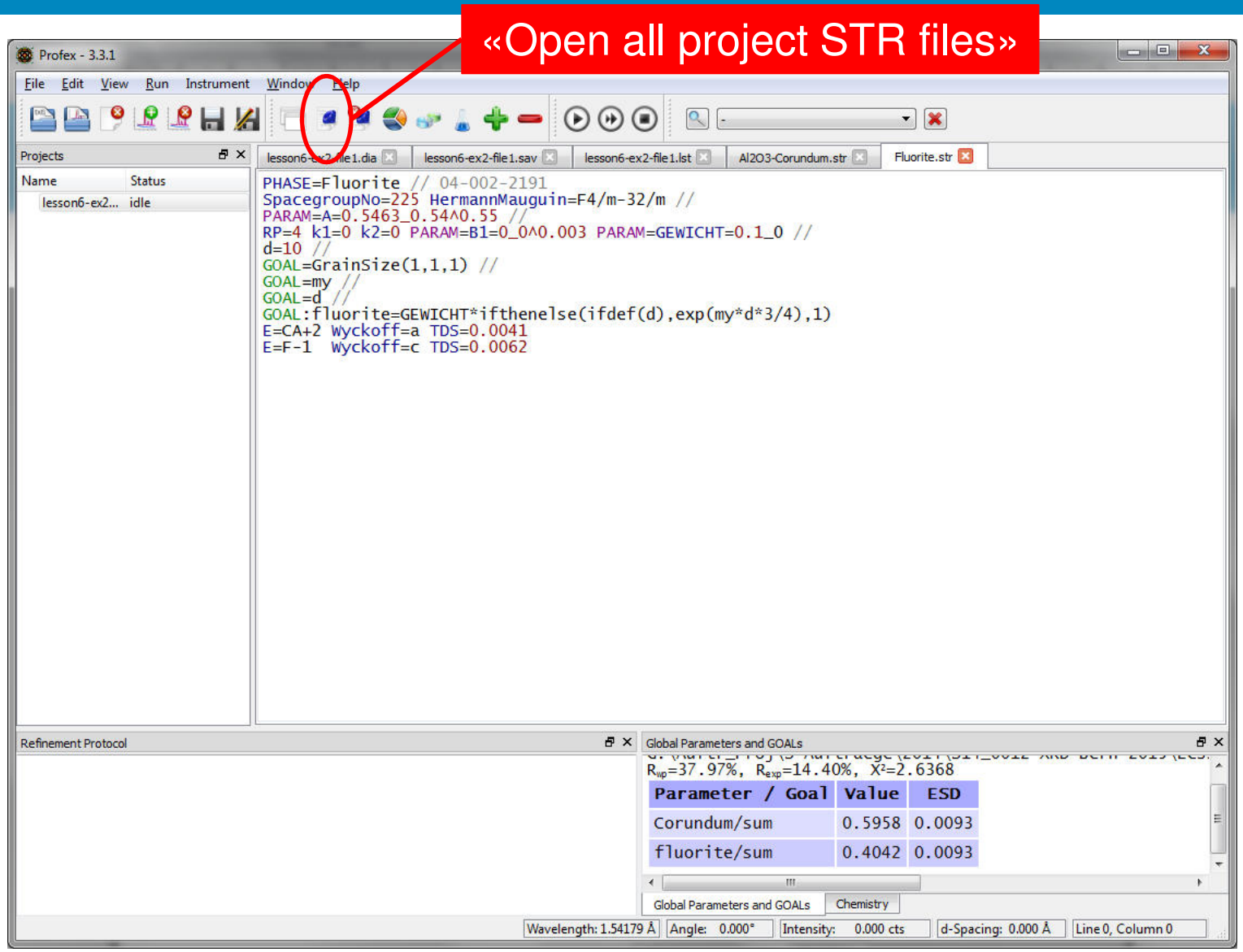
Integrated intensity: correct (?)

Peak-broadening: wrong

Specific for Fluorite phase.

Can be fixed in file «fluorite.str»

BGMN Structure Files (*.str)



BGMN Structure Files (*.str)

```
PHASE=Fluorite // 04-002-2191
SpacegroupNo=225 HermannMauguin=F4/m-32/m //
PARAM=A=0.5463_0.54^0.55 //
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.003 PARAM=GEWICHT=0.1_0 //
d=10 //
GOAL=GrainSize(1,1,1) //
GOAL=my //
GOAL=d //
GOAL:fluorite=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1)
E=CA+2 Wyckoff=a TDS=0.0041
E=F-1 Wyckoff=c TDS=0.0062
```

Phase name // Database reference

Space group number & H-M symbol

Unit Cell: *a* axis (nm)

Peak profile parameters

Mean particle size (µm), optional

Goals (optional, these values are reported in the results file)

List of atomic positions

Full notation:

E=CA+2(1) Wyckoff=a x=0.0 y=0.0 z=0.0 TDS=0.0041

Element

Wyckoff sequence

Thermal displacement parameter (B_{iso} [nm^2])

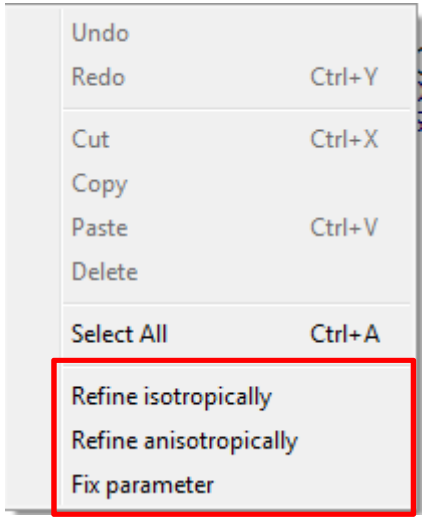
Site occupancy

Fractional coordinates

BGMN Structure Files (*.str)

```
PHASE=Fluorite // 04-002-2191
SpacegroupNo=225 HermannMauguin=F4/m-32/m //
PARAM=A=0.5463_0.54^0.55 //
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.003 PARAM=GEWICHT=0.1_0 //
d=10 //
GOAL=GrainSize(1,1,1) //
GOAL=my //
GOAL=d //
GOAL:fluorite=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1)
E=CA+2 Wyckoff=a TDS=0.0041
E=F-1 Wyckoff=c TDS=0.0062
```

Right mouse button on a parameter:



Fix parameter:	Refined parameter:	Refined parameter with limits:
A=0.5463	PARAM=A=0.5463	PARAM=A=0.5463_0.54^0.55
Name Value	Release for refinement Name Starting value	Release for refinement Name Starting value Lower limit Upper limit

Lesson 6: Example 2

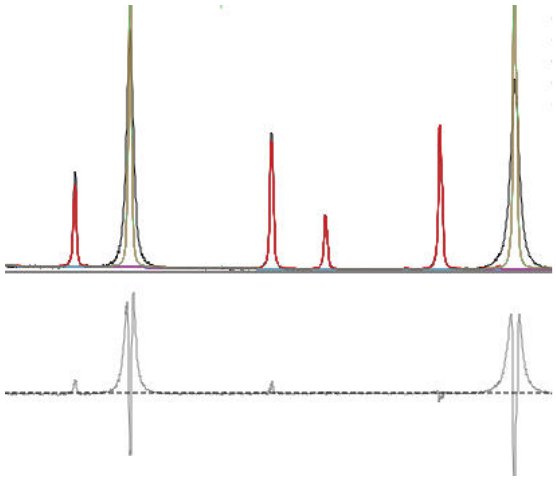
```
PHASE=Fluorite // 04-002-2191
SpacegroupNo=225 HermannMauguin=F4/m-32/m //
PARAM=A=0.5463_0.54^0.55 //
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.003 PARAM=GEWICHT=0.1_0 //
d=10 //
GOAL=GrainSize(1,1,1) //
GOAL=my //
GOAL=d //
GOAL:fluorite=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1)
E=CA+2 Wyckoff=a TDS=0.0041
E=F-1 Wyckoff=c TDS=0.0062
```

In Lesson 6, Example 2, peak broadening was not fitted correctly

Peak shape is controlled here

B1: peak broadening caused by crystallite size

k2: peak broadening caused by micro-strain



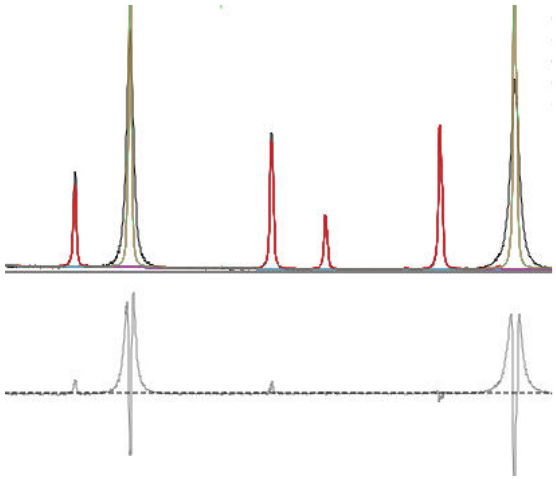
See http://www.bgmn.de/variables.html#real for RP=4 and k1=0

Lesson 6: Example 2

```
PHASE=Fluorite // 04-002-2191
SpacegroupNo=225 HermannMauguin=F4/m-32/m //
PARAM=A=0.5463_0.54^0.55 //
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.003 PARAM=GEWICHT=0.1_0 //
d=10 //
GOAL=GrainSize(1,1,1) //
GOAL=my //
GOAL=d //
GOAL:fluorite=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1)
E=CA+2 Wyckoff=a TDS=0.0041
E=F-1 Wyckoff=c TDS=0.0062
```

B1: refined, but limited to the range 0.000 – 0.003 (upper limit may be too strict)

k2: micro strain effect, not refined (necessary?)



Lesson 6: Example 2

Change:

```
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.003 PARAM=GEWICHT=0.1_0 //
```

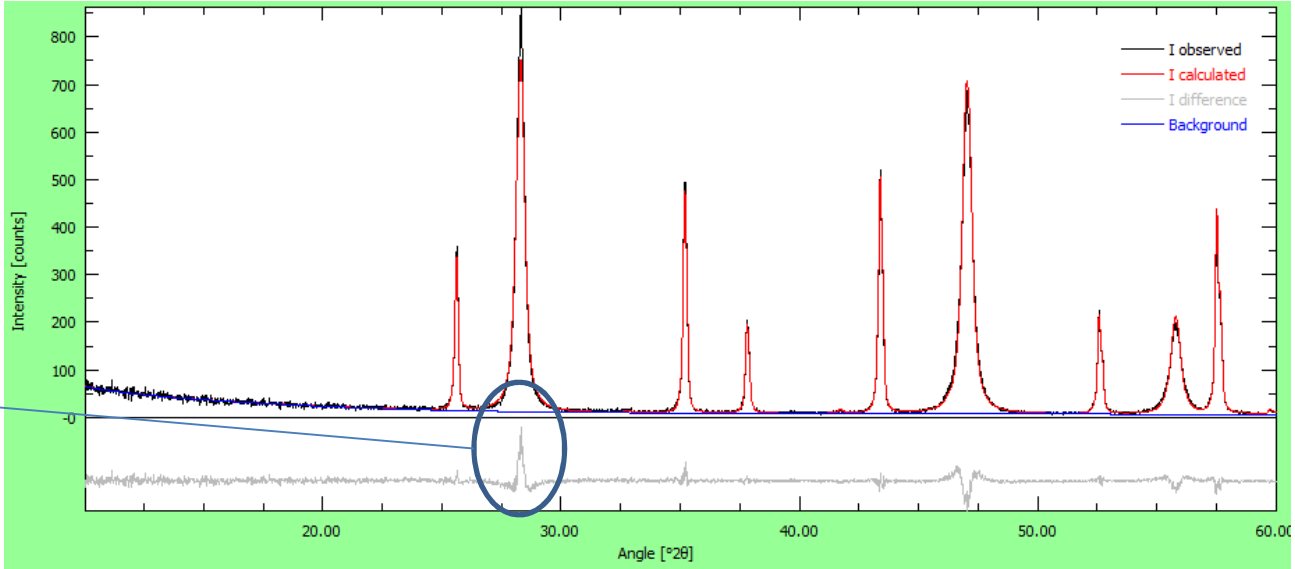
To:

```
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.03 PARAM=GEWICHT=0.1_0 //
```

Repeat Refinement

Better, but not perfect.

Is there microstrain?



Lesson 6: Example 2

Change:

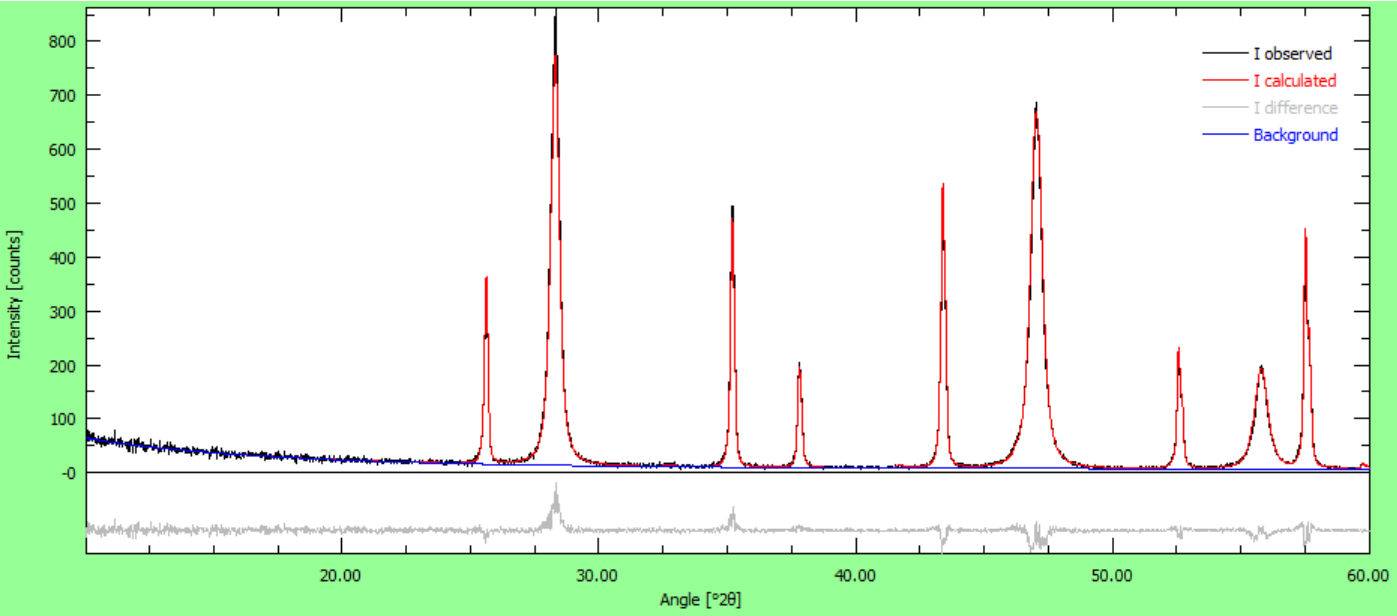
```
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.03 PARAM=GEWICHT=0.1_0 //
```

To:

```
RP=4 k1=0 PARAM=k2=0_0 PARAM=B1=0_0^0.03 PARAM=GEWICHT=0.1_0 //
```

Repeat Refinement

Better, but still not perfect.



Lesson 6: Example 2

Preferred Orientation / Texture:

- Refine «GEWICHT» anisotropically:
  - Right mouse button on GEWICHT
  - «Refine anisotropically»

Changes:

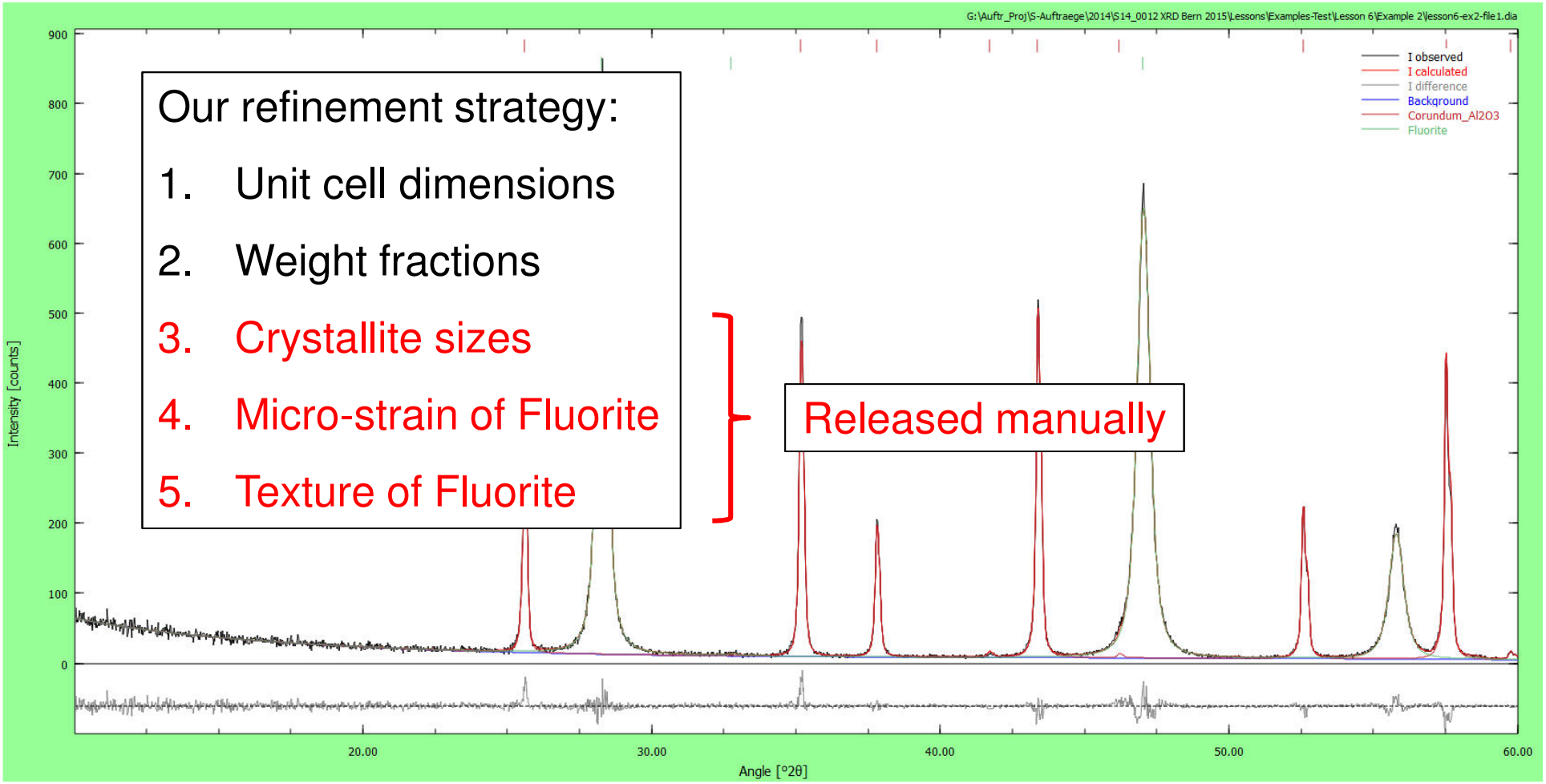
```
RP=4 k1=0 PARAM=k2=0_0 PARAM=B1=0_0^0.03 PARAM=GEWICHT=0.1_0 //
```

To:

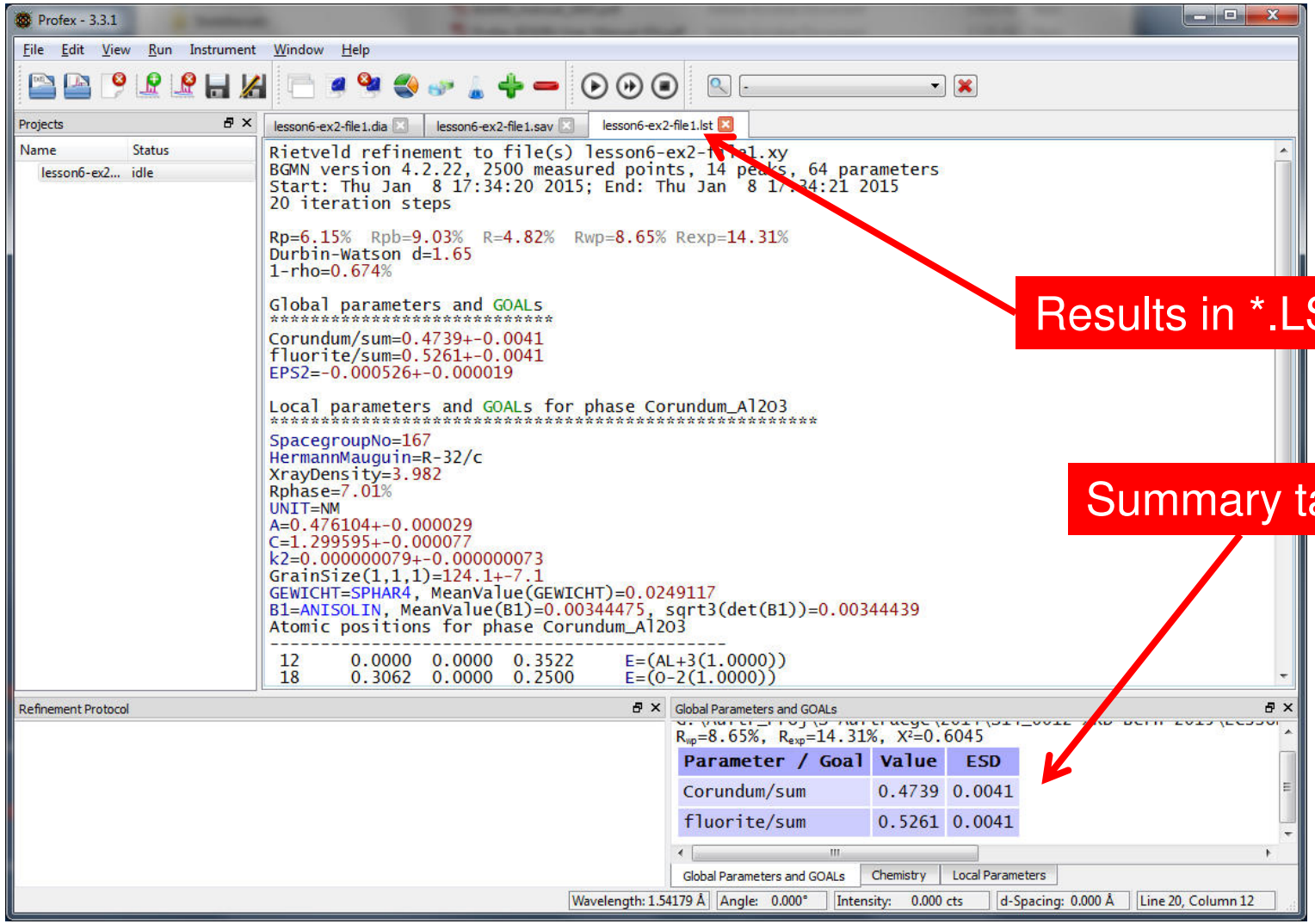
```
RP=4 k1=0 PARAM=k2=0_0 PARAM=B1=0_0^0.03 GEWICHT=SPHAR4 //
```

Repeat Refinement

Lesson 6: Example 2



Lesson 6: Example 2



Summary: Structure Files (*.str)

- Structure file database (*.str) is stored in …\Profex-BGMN-Bundle-3.3.1\Profex\Structures
- Copied by Profex to the location of the scan file
- They contain:
  - Space group information
  - Unit cell dimensions
  - Profile parameters
  - Scaling (weight fraction)
  - List of atoms (element, SOF, Wyckoff sequence, fract. coordinates, TDS)
  - Optional «Goals»: Results / values printed to the results file (*.lst)
- Release parameters for refinement:
  - «PARAM=»
  - Optionally (recommended!): «_lowerLimit» and «^upperLimit»

Summary: Structure Files (*.str)

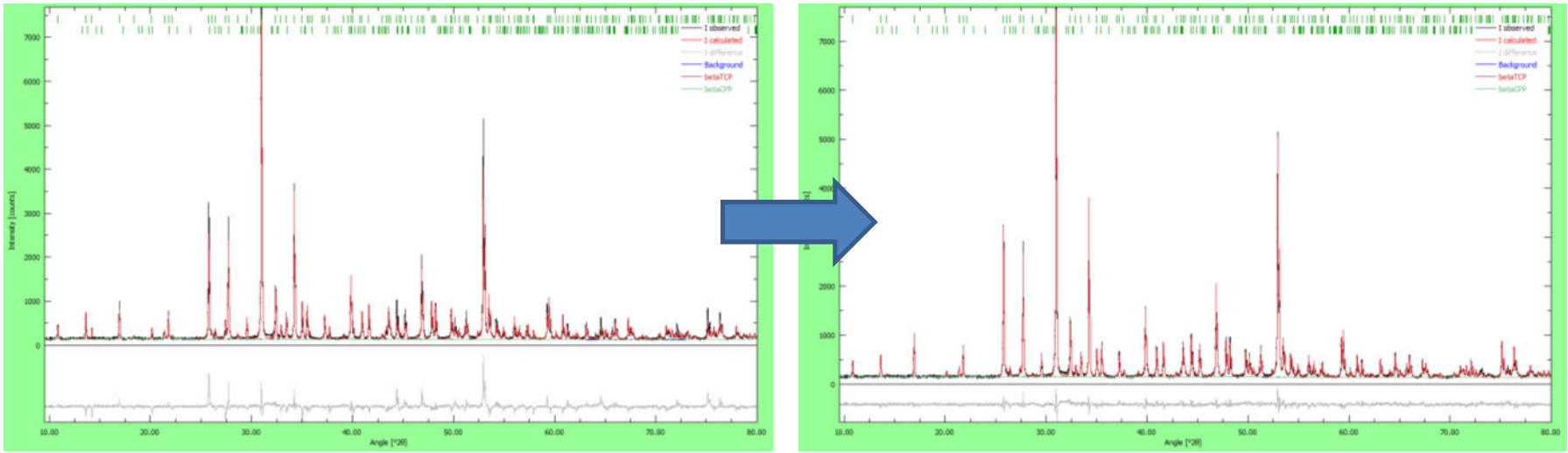
Refinements are «fine tuned» by editing Structure Files:

Commonly:

- Set reasonable upper and lower limits
- Control peak broadening
- Control texture / preferred orientation

Rarely:

- Control structural parameters:
  - atomic coordinates
  - site occupancies
  - thermal displacement parameters



Structure Databases

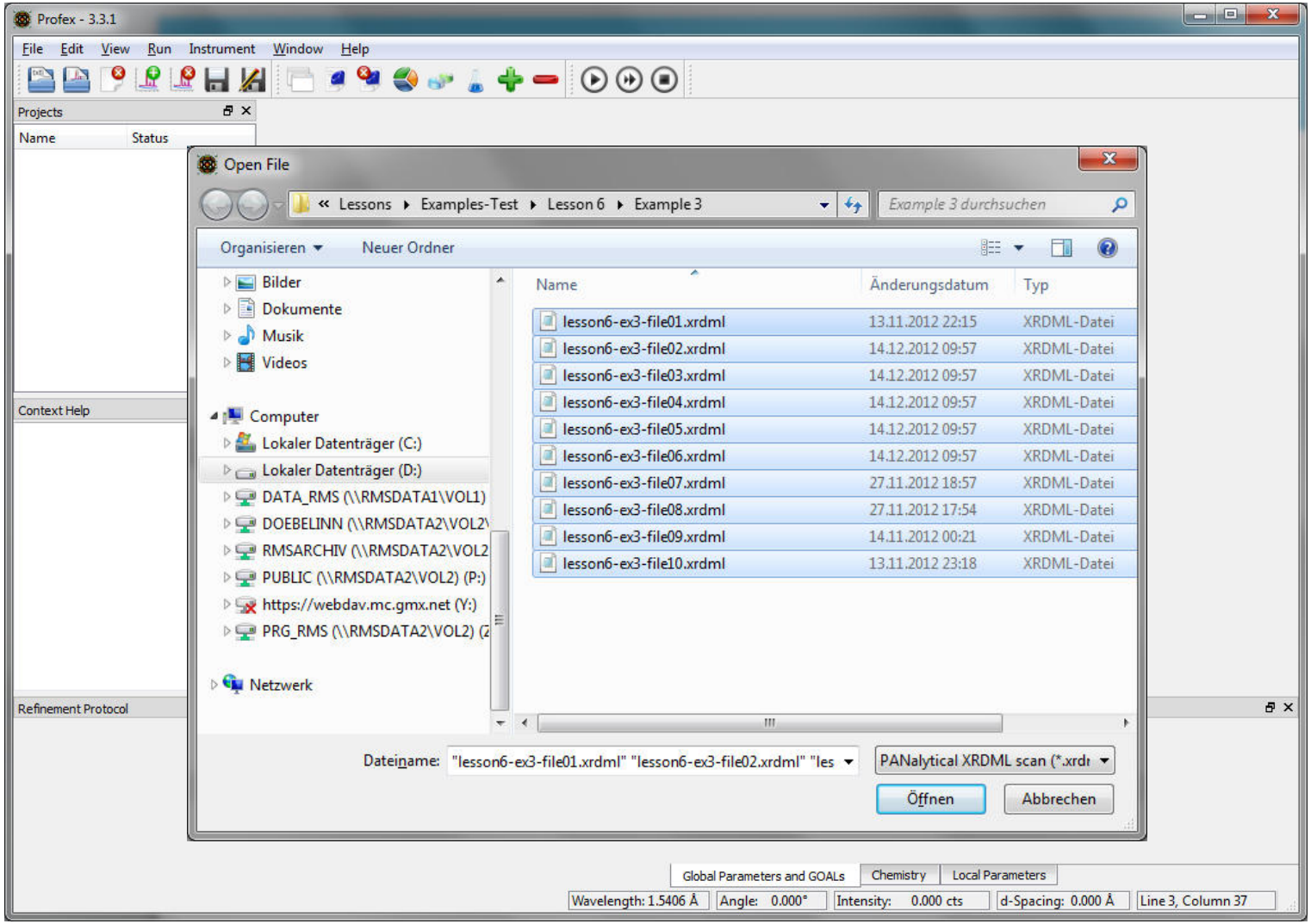
STR files included in Profex bundle
(created manually by Nicola Doebelin)

http://www.bgmn.de/download-structures.html

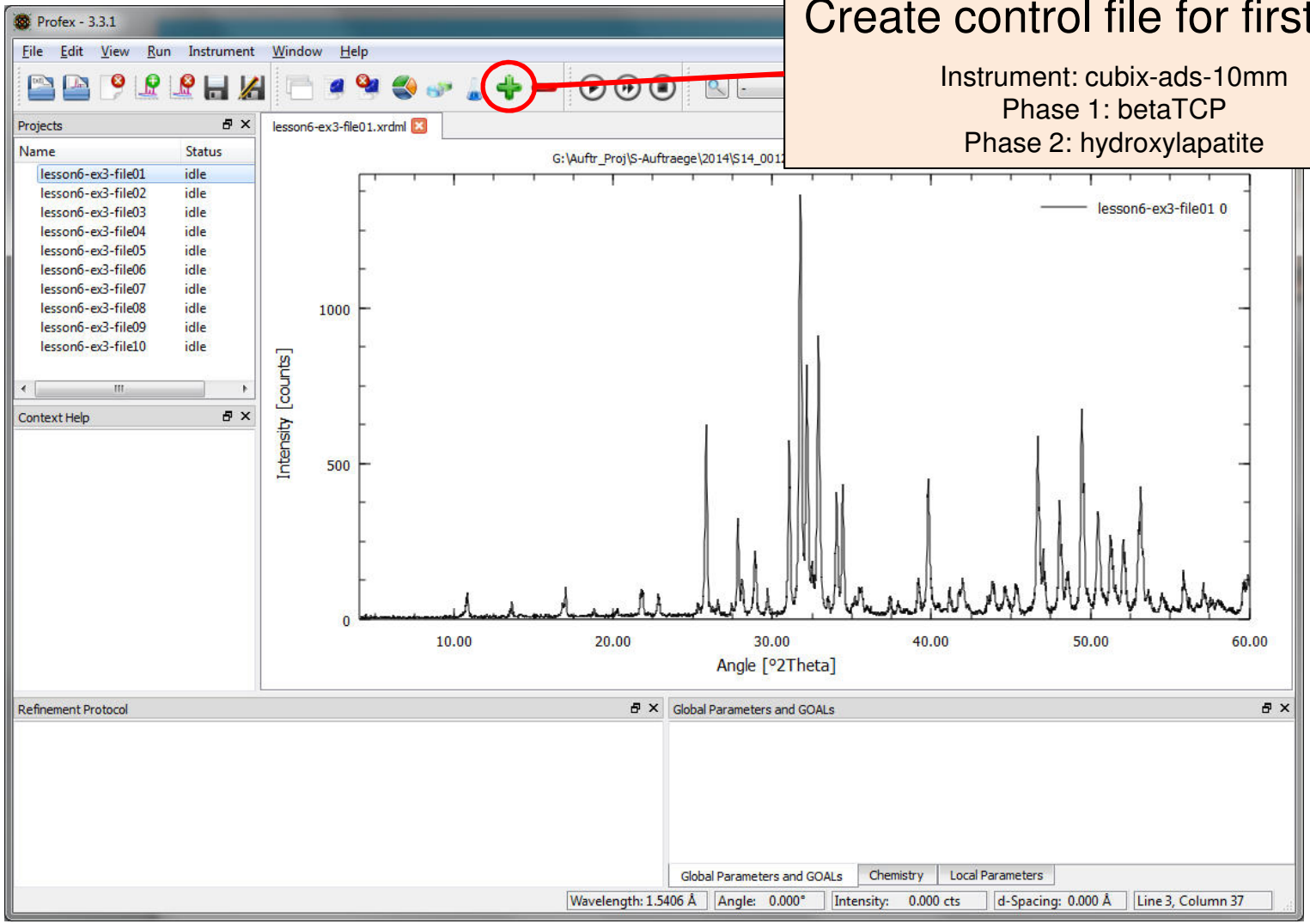
More on Structure Files:

Lesson 8: Creating Structure Files

Lesson 6: Example 3 - Batch Refinement



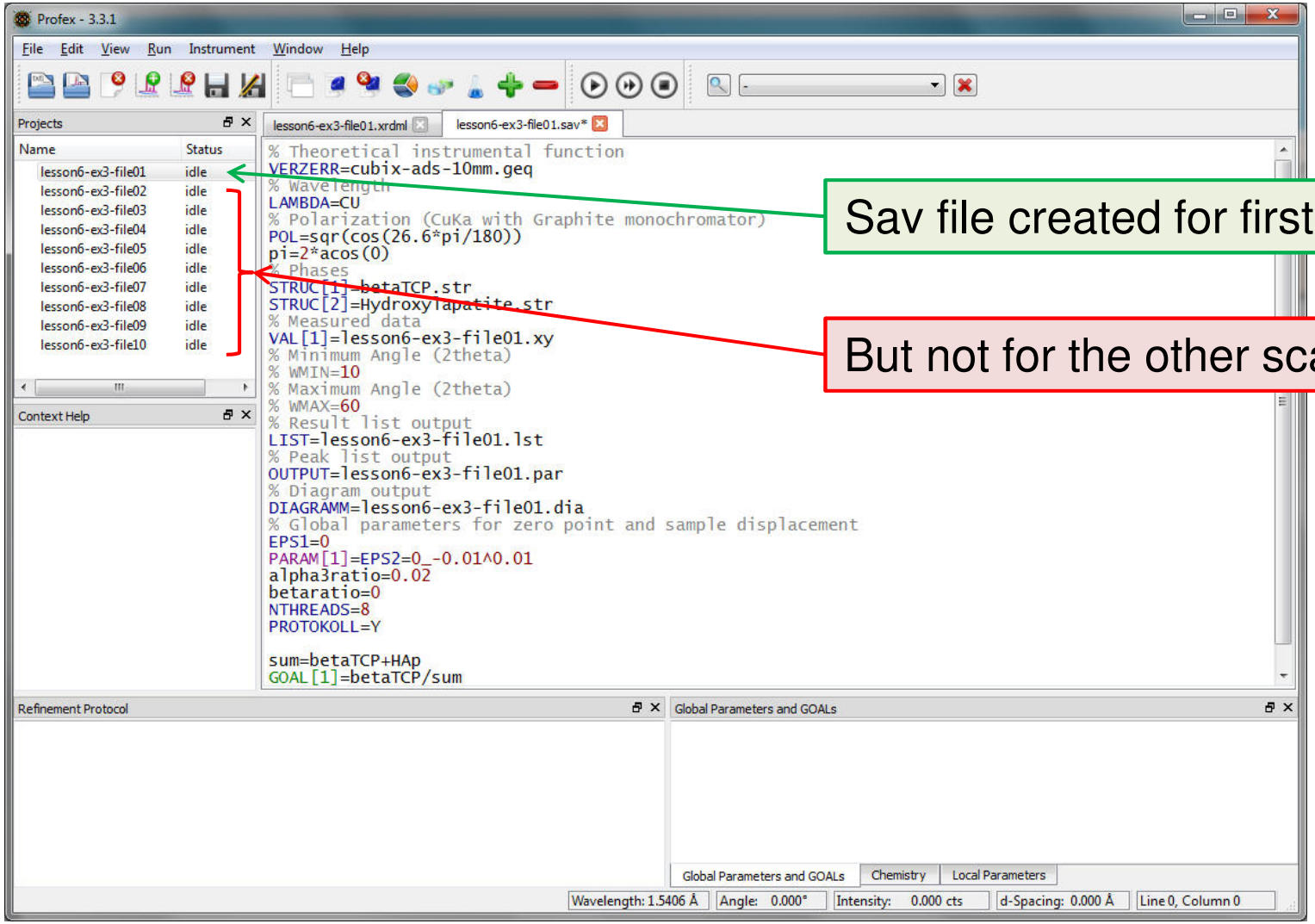
Lesson 6: Example 3 - Batch Refinement



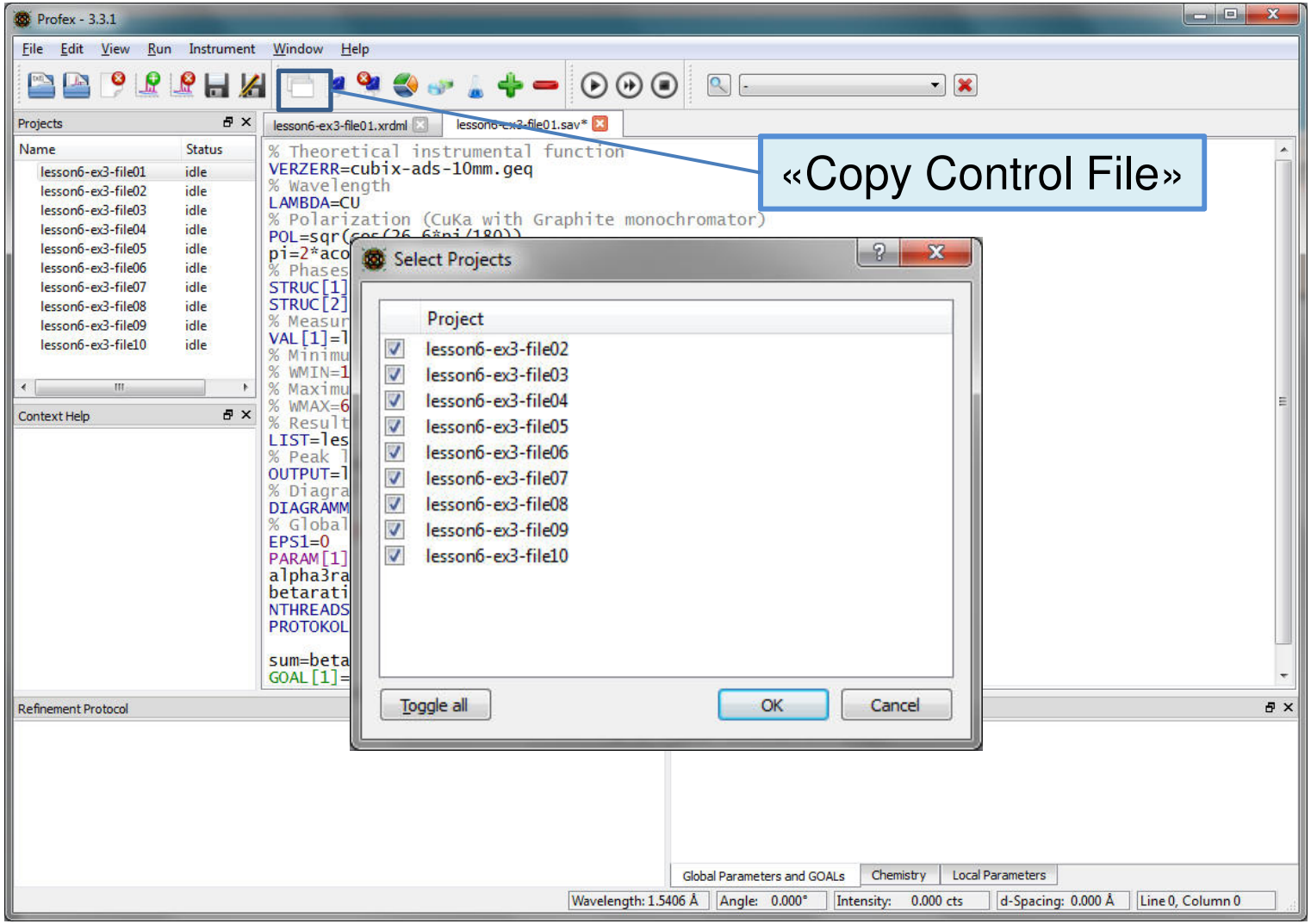
Create control file for first scan

Instrument: cubix-ads-10mm
Phase 1: betaTCP
Phase 2: hydroxylapatite

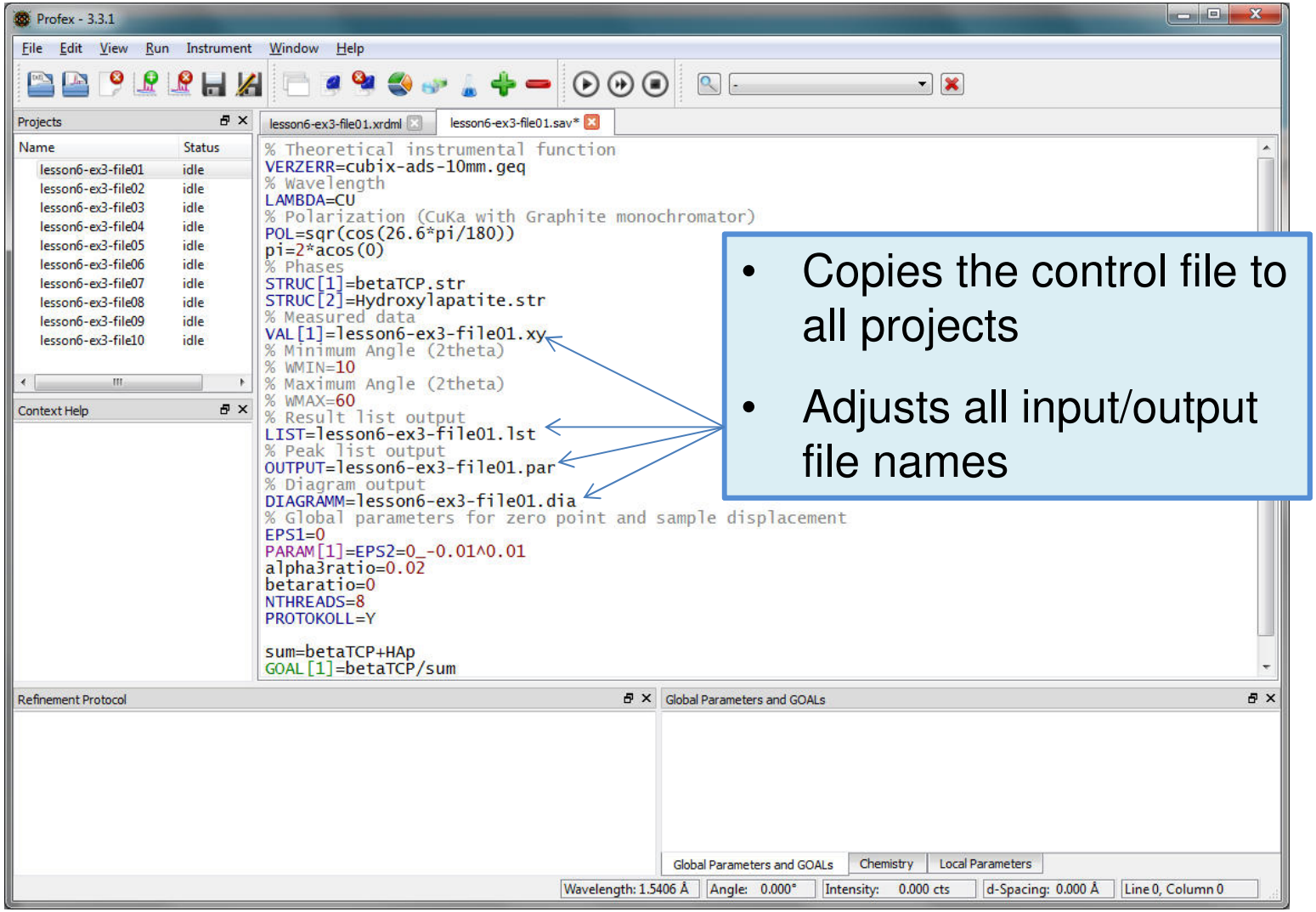
Lesson 6: Example 3 - Batch Refinement



Lesson 6: Example 3 - Batch Refinement

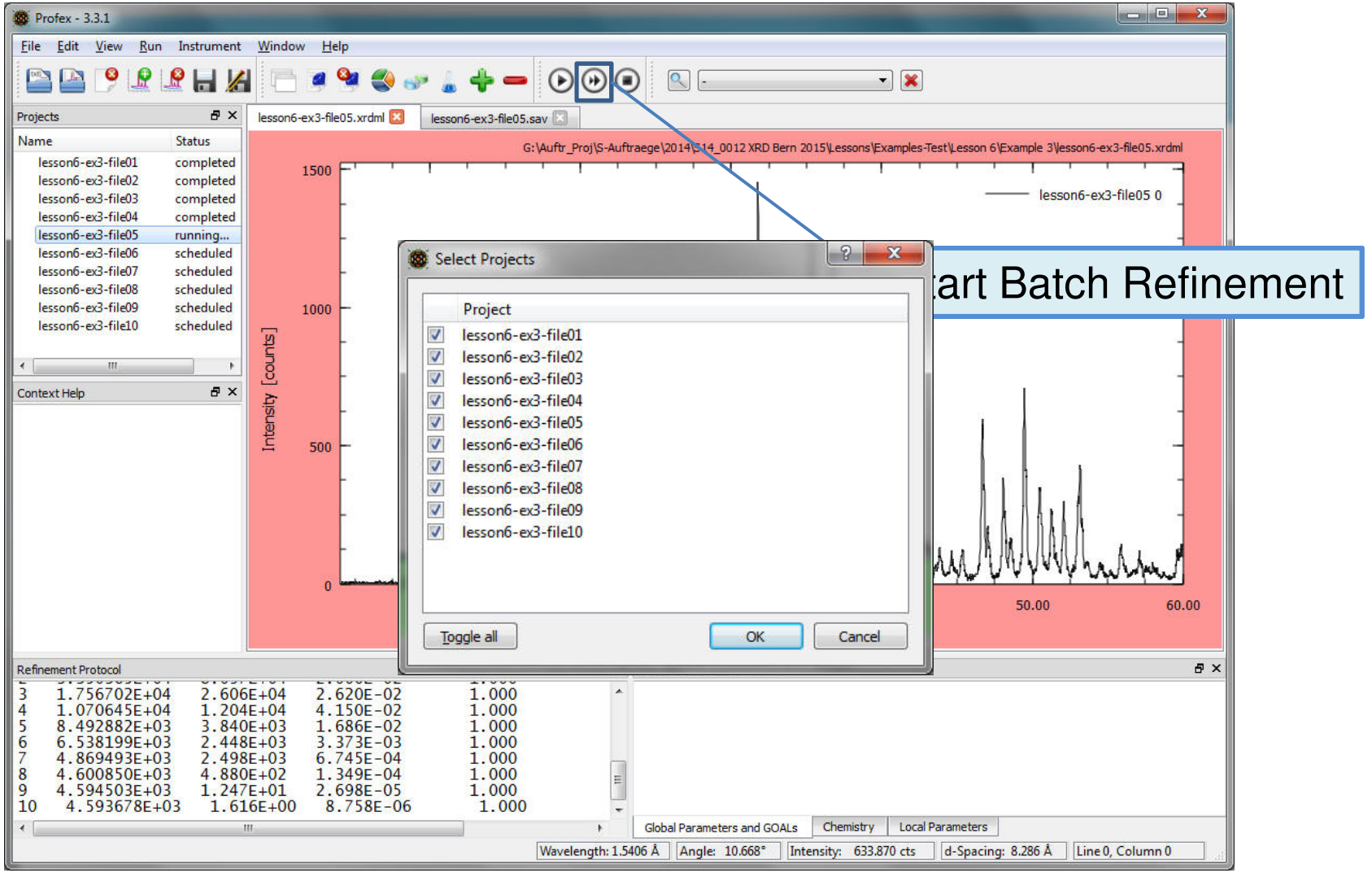


Lesson 6: Example 3 - Batch Refinement

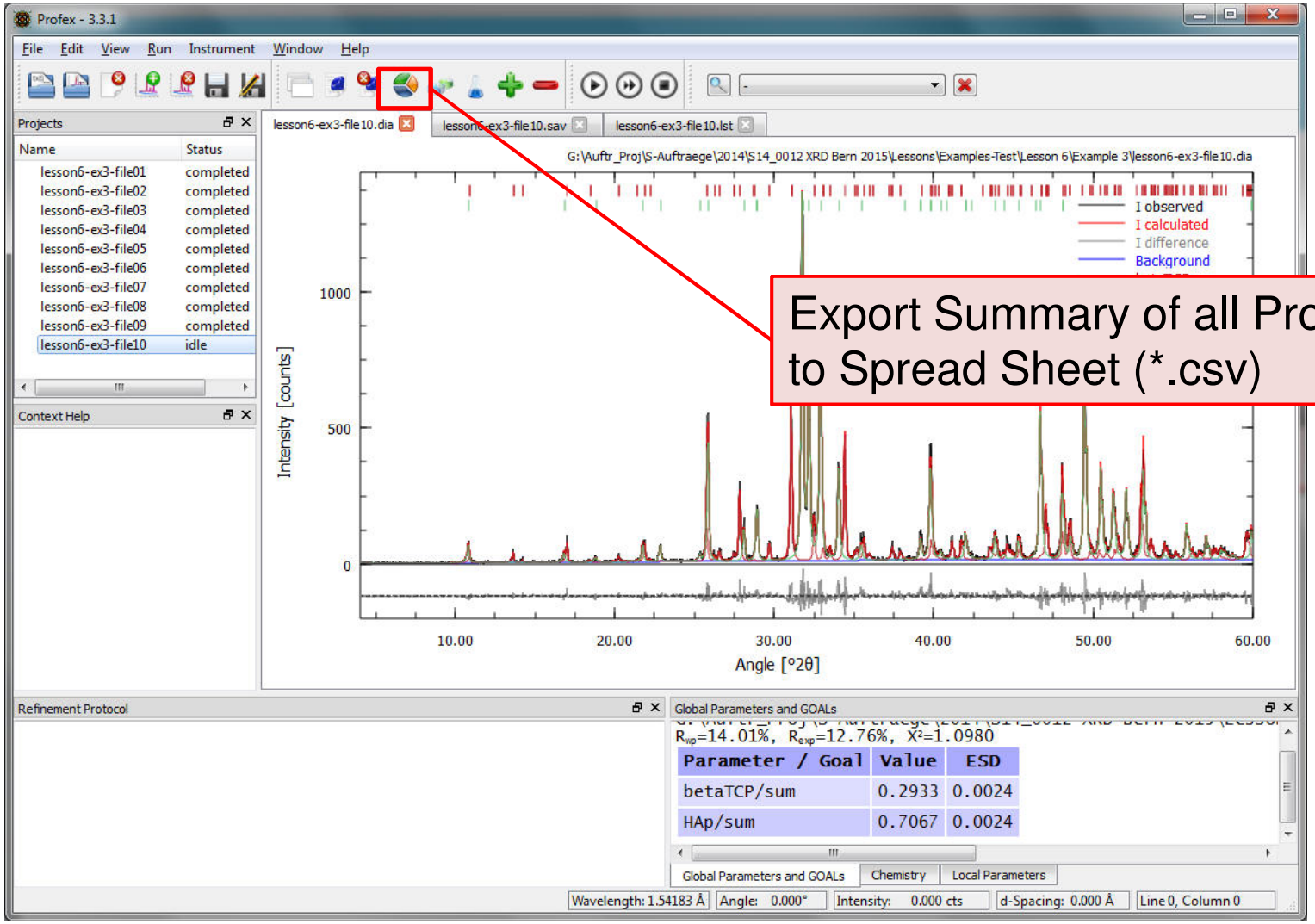


- Copies the control file to all projects
- Adjusts all input/output file names

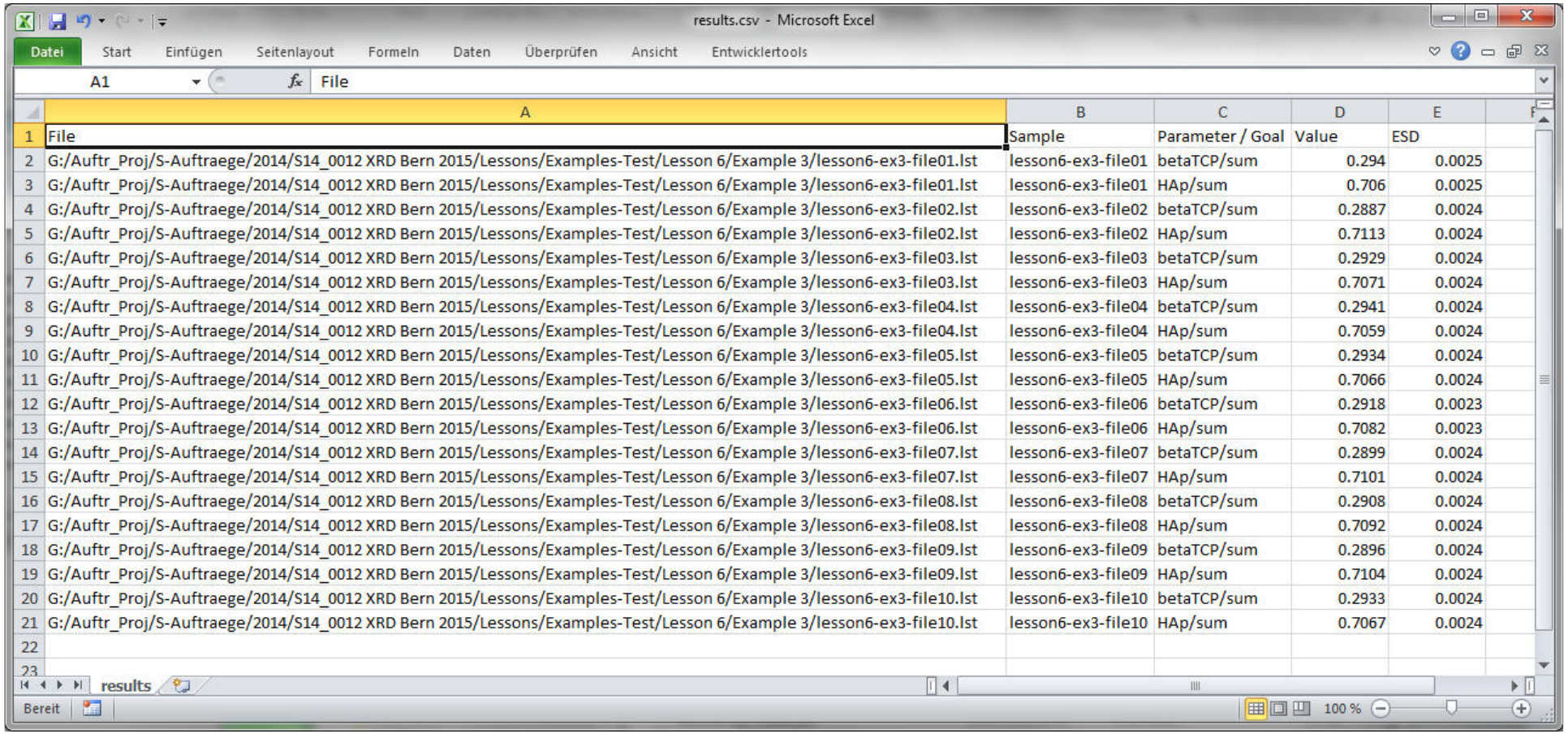
Lesson 6: Example 3 - Batch Refinement



Lesson 6: Example 3 - Batch Refinement

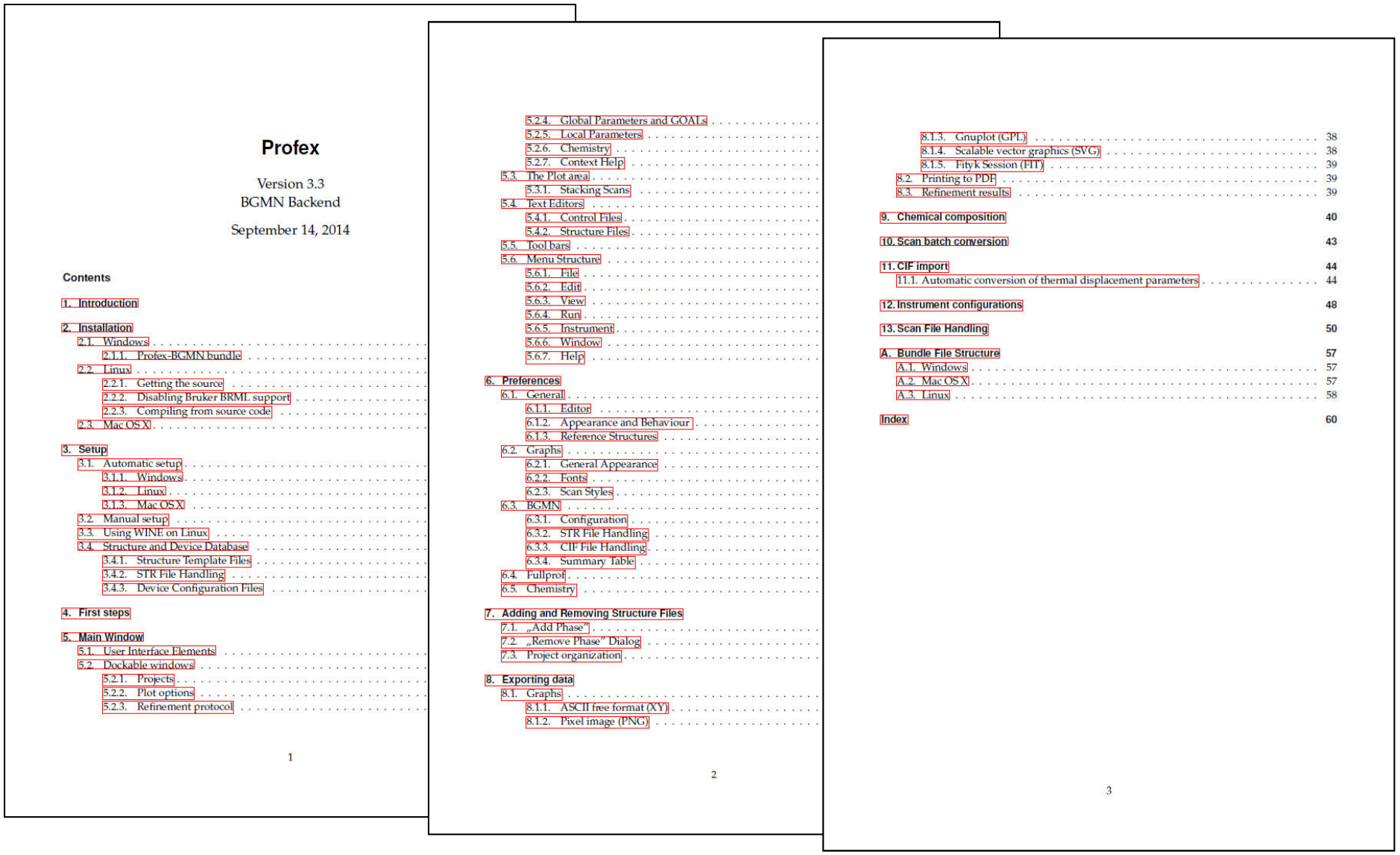


Lesson 6: Example 3 - Batch Refinement



	A	B	C	D	E
1	File	Sample	Parameter / Goal	Value	ESD
2	G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file01.lst	lesson6-ex3-file01	betaTCP/sum	0.294	0.0025
3	G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file01.lst	lesson6-ex3-file01	HAp/sum	0.706	0.0025
4	G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file02.lst	lesson6-ex3-file02	betaTCP/sum	0.2887	0.0024
5	G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file02.lst	lesson6-ex3-file02	HAp/sum	0.7113	0.0024
6	G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file03.lst	lesson6-ex3-file03	betaTCP/sum	0.2929	0.0024
7	G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file03.lst	lesson6-ex3-file03	HAp/sum	0.7071	0.0024
8	G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file04.lst	lesson6-ex3-file04	betaTCP/sum	0.2941	0.0024
9	G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file04.lst	lesson6-ex3-file04	HAp/sum	0.7059	0.0024
10	G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file05.lst	lesson6-ex3-file05	betaTCP/sum	0.2934	0.0024
11	G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file05.lst	lesson6-ex3-file05	HAp/sum	0.7066	0.0024
12	G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file06.lst	lesson6-ex3-file06	betaTCP/sum	0.2918	0.0023
13	G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file06.lst	lesson6-ex3-file06	HAp/sum	0.7082	0.0023
14	G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file07.lst	lesson6-ex3-file07	betaTCP/sum	0.2899	0.0024
15	G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file07.lst	lesson6-ex3-file07	HAp/sum	0.7101	0.0024
16	G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file08.lst	lesson6-ex3-file08	betaTCP/sum	0.2908	0.0024
17	G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file08.lst	lesson6-ex3-file08	HAp/sum	0.7092	0.0024
18	G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file09.lst	lesson6-ex3-file09	betaTCP/sum	0.2896	0.0024
19	G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file09.lst	lesson6-ex3-file09	HAp/sum	0.7104	0.0024
20	G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file10.lst	lesson6-ex3-file10	betaTCP/sum	0.2933	0.0024
21	G:/Auftr_Proj/S-Auftraege/2014/S14_0012 XRD Bern 2015/Lessons/Examples-Test/Lesson 6/Example 3/lesson6-ex3-file10.lst	lesson6-ex3-file10	HAp/sum	0.7067	0.0024
22					
23					

User Manual



Profex

Version 3.3
BGMN Backend

September 14, 2014

Contents

1. Introduction

2. Installation
   2.1. Windows
      2.1.1. Profex-BGMN bundle
   2.2. Linux
      2.2.1. Getting the source
      2.2.2. Disabling Bruker BRML support
      2.2.3. Compiling from source code
   2.3. Mac OS X

3. Setup
   3.1. Automatic setup
      3.1.1. Windows
      3.1.2. Linux
      3.1.3. Mac OS X
   3.2. Manual setup
   3.3. Using WINE on Linux
   3.4. Structure and Device Database
      3.4.1. Structure Template Files
      3.4.2. STR File Handling
      3.4.3. Device Configuration Files

4. First steps

5. Main Window
   5.1. User Interface Elements
   5.2. Dockable windows
      5.2.1. Projects
      5.2.2. Plot options
      5.2.3. Refinement protocol
      5.2.4. Global Parameters and GOALs
      5.2.5. Local Parameters
      5.2.6. Chemistry
      5.2.7. Context Help
   5.3. The Plot area
      5.3.1. Stacking Scans
   5.4. Text Editors
      5.4.1. Control Files
      5.4.2. Structure Files
   5.5. Tool bars
   5.6. Menu Structure
      5.6.1. File
      5.6.2. Edit
      5.6.3. View
      5.6.4. Run
      5.6.5. Instrument
      5.6.6. Window
      5.6.7. Help

6. Preferences
   6.1. General
      6.1.1. Editor
      6.1.2. Appearance and Behaviour
      6.1.3. Reference Structures
   6.2. Graphs
      6.2.1. General Appearance
      6.2.2. Fonts
      6.2.3. Scan Styles
   6.3. BGMN
      6.3.1. Configuration
      6.3.2. STR File Handling
      6.3.3. CIF File Handling
      6.3.4. Summary Table
   6.4. Fullprof
   6.5. Chemistry

7. Adding and Removing Structure Files
   7.1. „Add Phase"
   7.2. „Remove Phase" Dialog
   7.3. Project organization

8. Exporting data
   8.1. Graphs
      8.1.1. ASCII free format (XY)
      8.1.2. Pixel image (PNG)
      8.1.3. Gnuplot (GPL) 38
      8.1.4. Scalable vector graphics (SVG) 38
      8.1.5. Fityk Session (FIT) 39
   8.2. Printing to PDF 39
   8.3. Refinement results 39

9. Chemical composition 40

10. Scan batch conversion 43

11. CIF import 44
   11.1. Automatic conversion of thermal displacement parameters 44

12. Instrument configurations 48

13. Scan File Handling 50

A. Bundle File Structure 57
   A.1. Windows 57
   A.2. Mac OS X 57
   A.3. Linux 58

Index 60