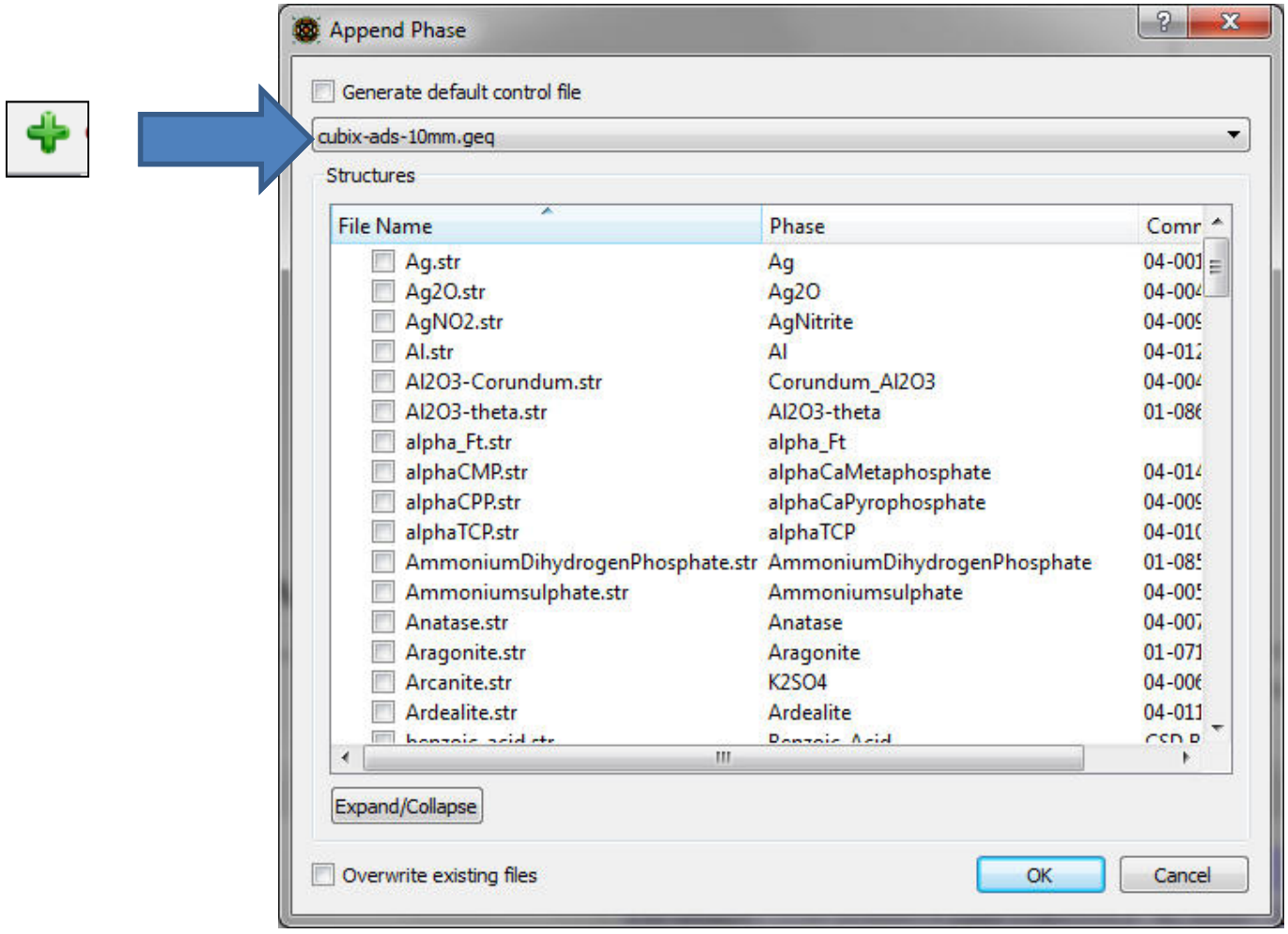
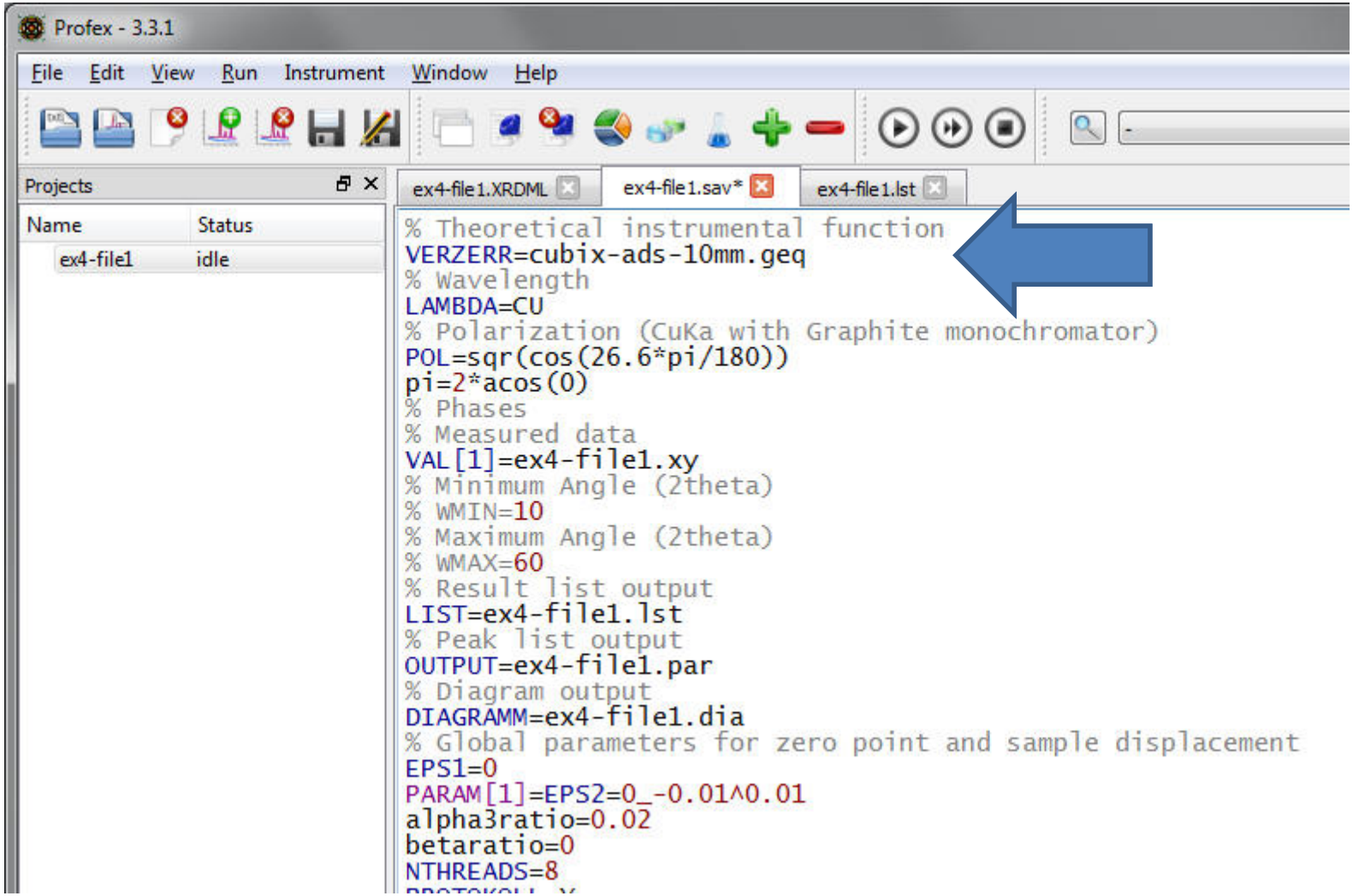
Lesson 9
Instrument Configuration Files

Nicola Döbelin
RMS Foundation, Bettlach, Switzerland

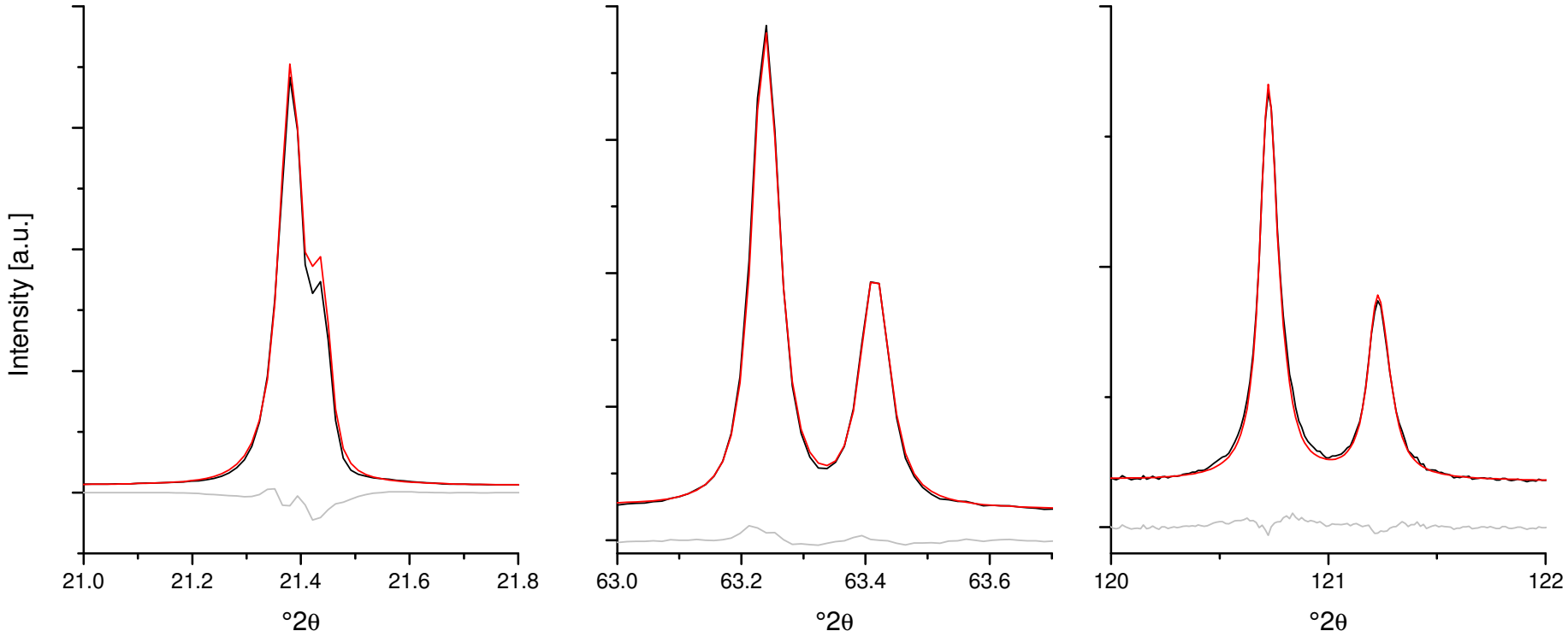
Instrument configuration file



Instrument configuration file



Fundamental Parameters Approach



Description of the peak profile

Instrument Configuration Files

Create / edit manually

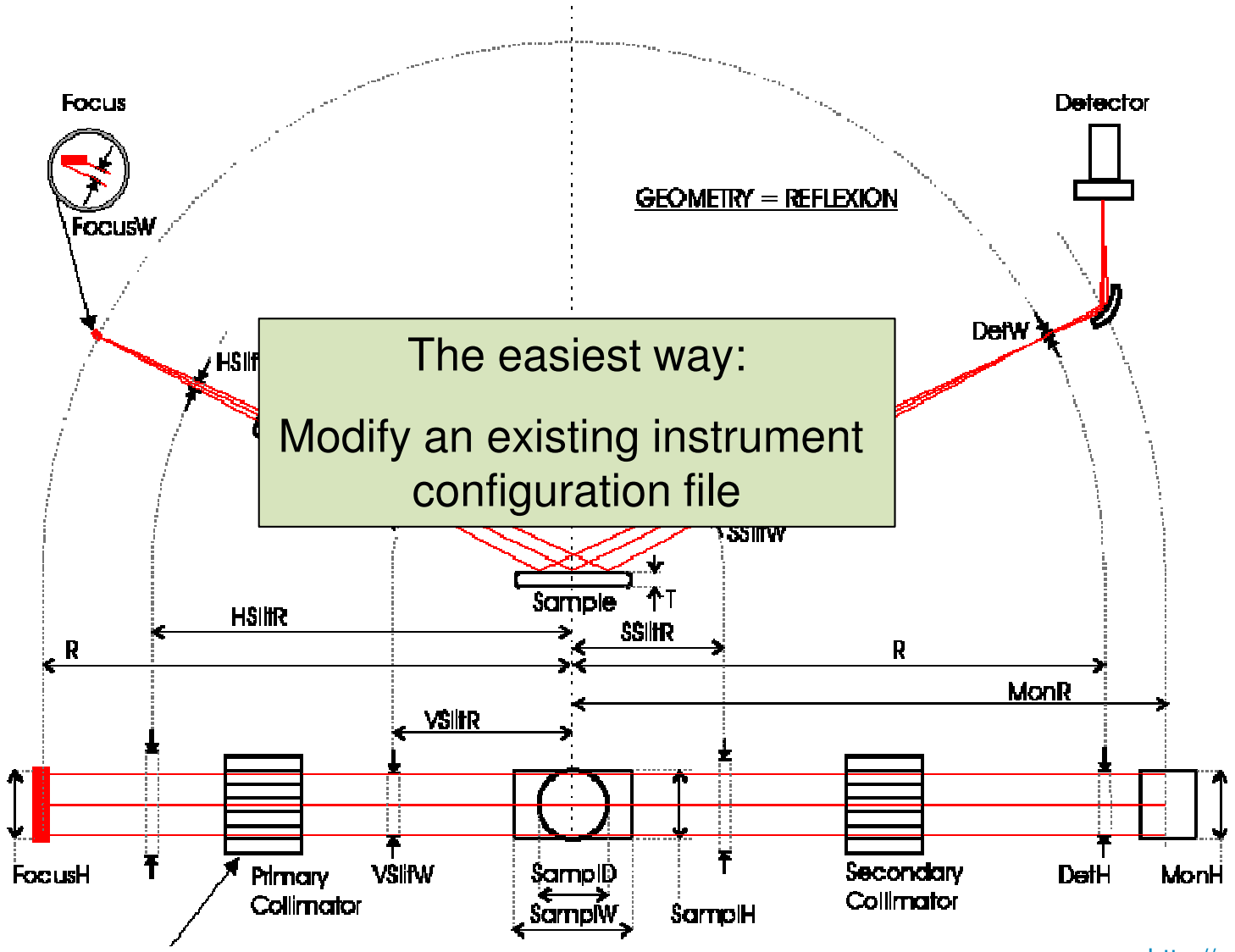
File	Description
Instrument.sav	Description of the instrument configuration
Instrument.ger	Calculated profile
Instrument.geq	Interpolated profile
Instrument.tpl	Template for *.sav control file for this configuration[1)] (Empty *.sav file)

All these files are stored in

…\Profex-BGMN-Bundle-3.3.1\Profex\Devices

[1)] Optional, only used by Profex, not required for BGMN

Instrument Configuration Files



http://www.bgmn.de

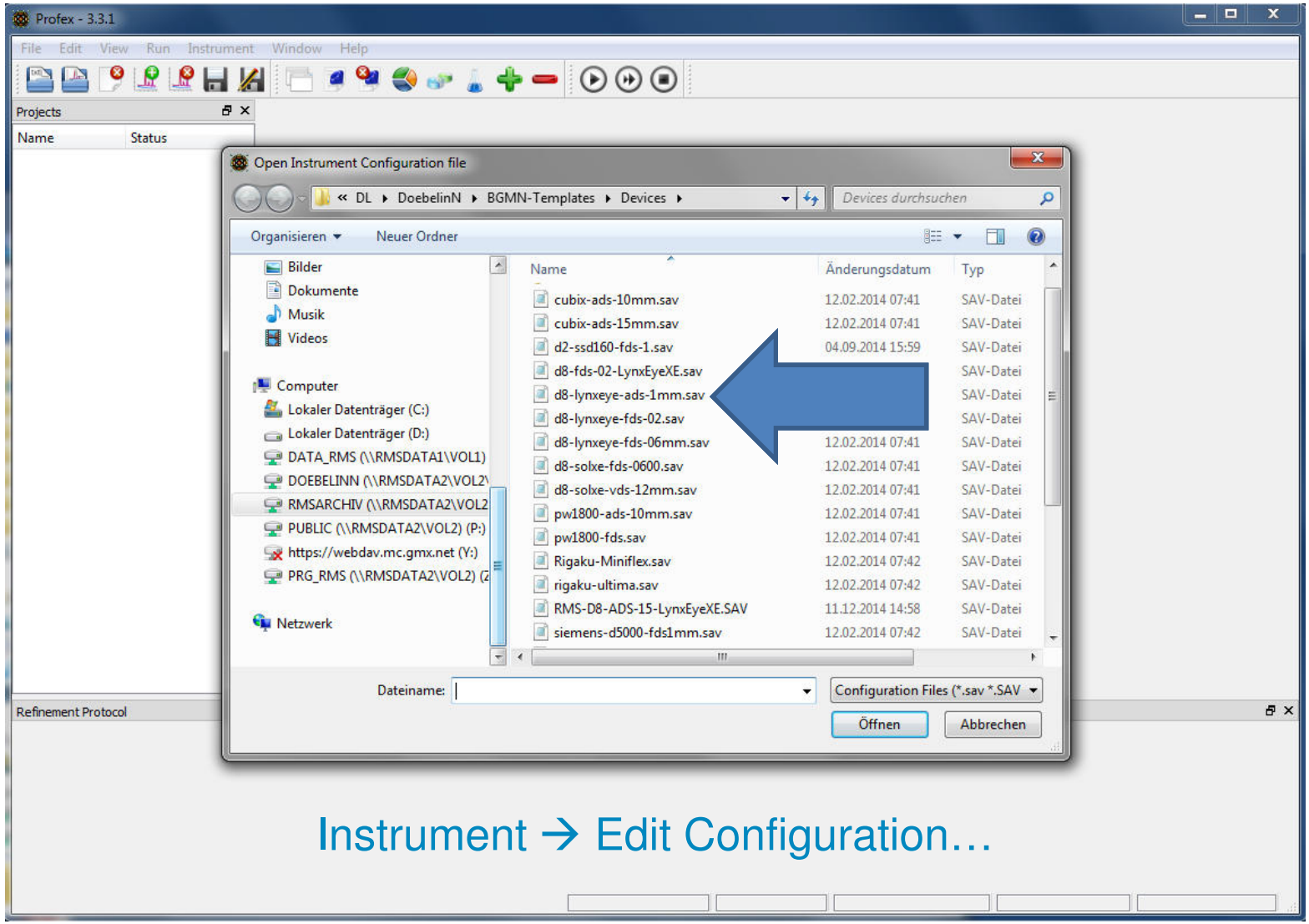
Editing Instrument Files

- Try to find an instrument configuration with…
  - … the same manufacturer
  - … the same model
  - … the same detector
  - … the same divergence slit mode (FDS / ADS)

Example	Your instrument:	Bruker D8 Advance
		LynxEye detector
		Automatic Divergence Slit

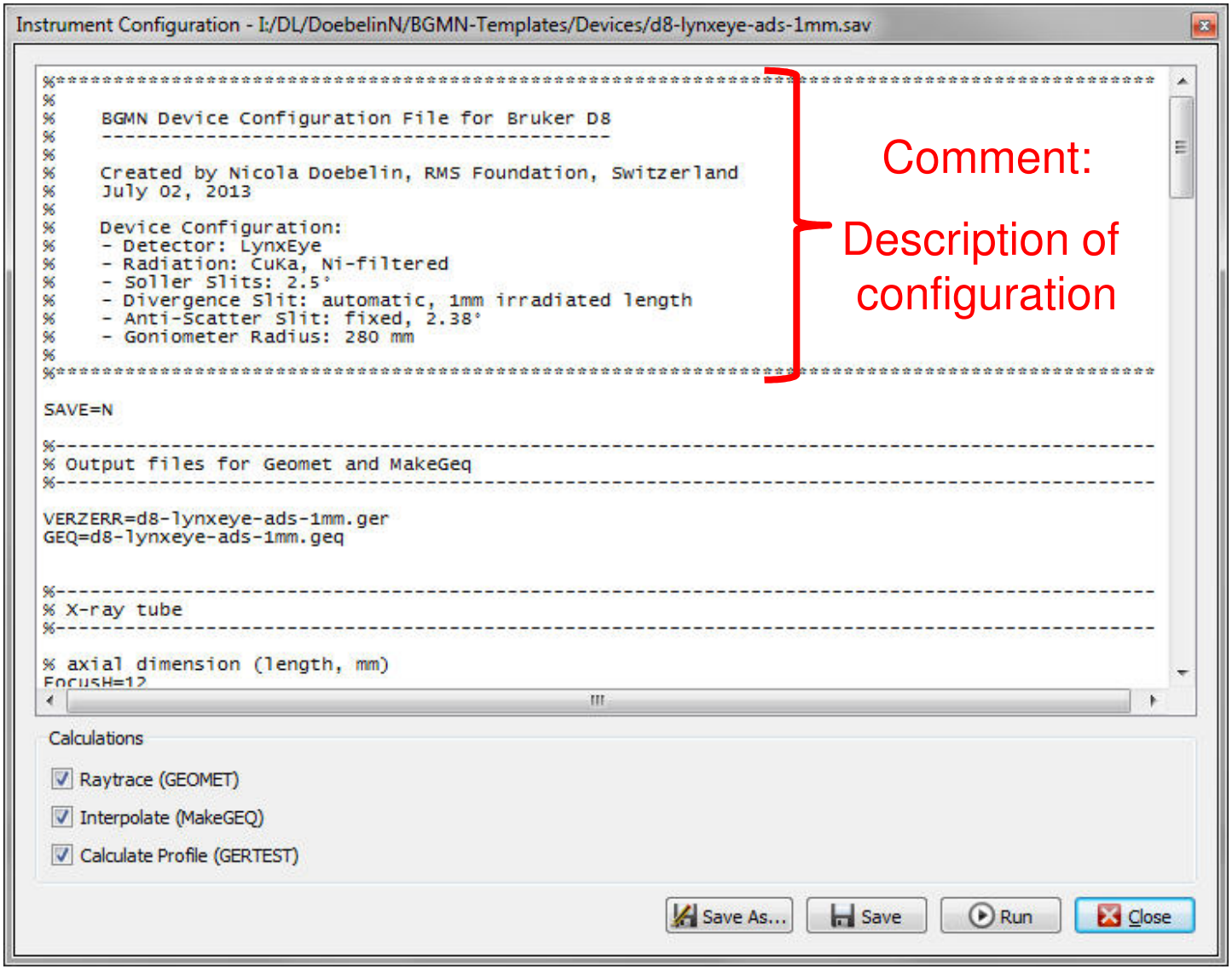
Modify configuration «d8-lynxeye-ads-1mm.sav»

Editing Instrument Files

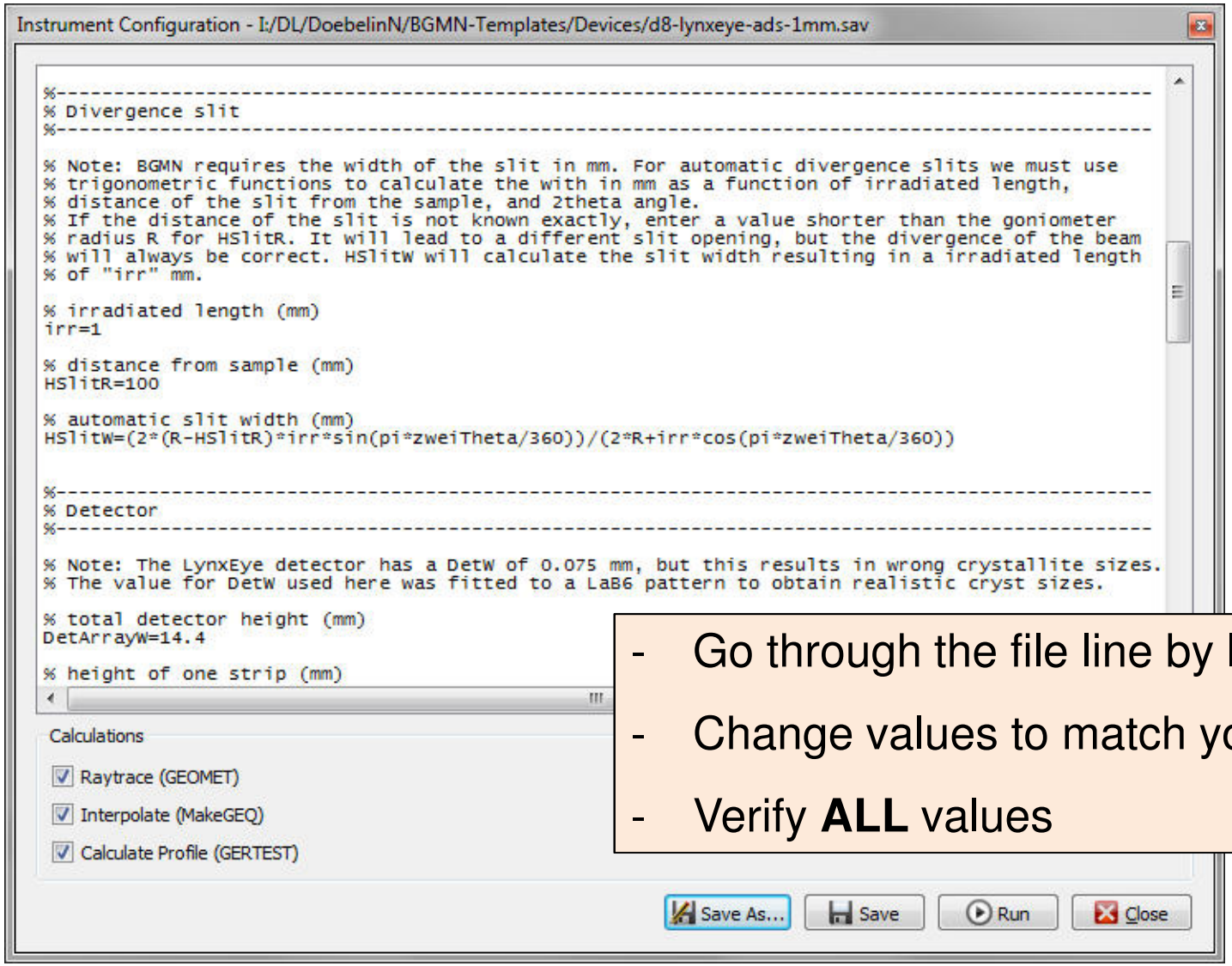


Instrument → Edit Configuration…

Editing Instrument Files

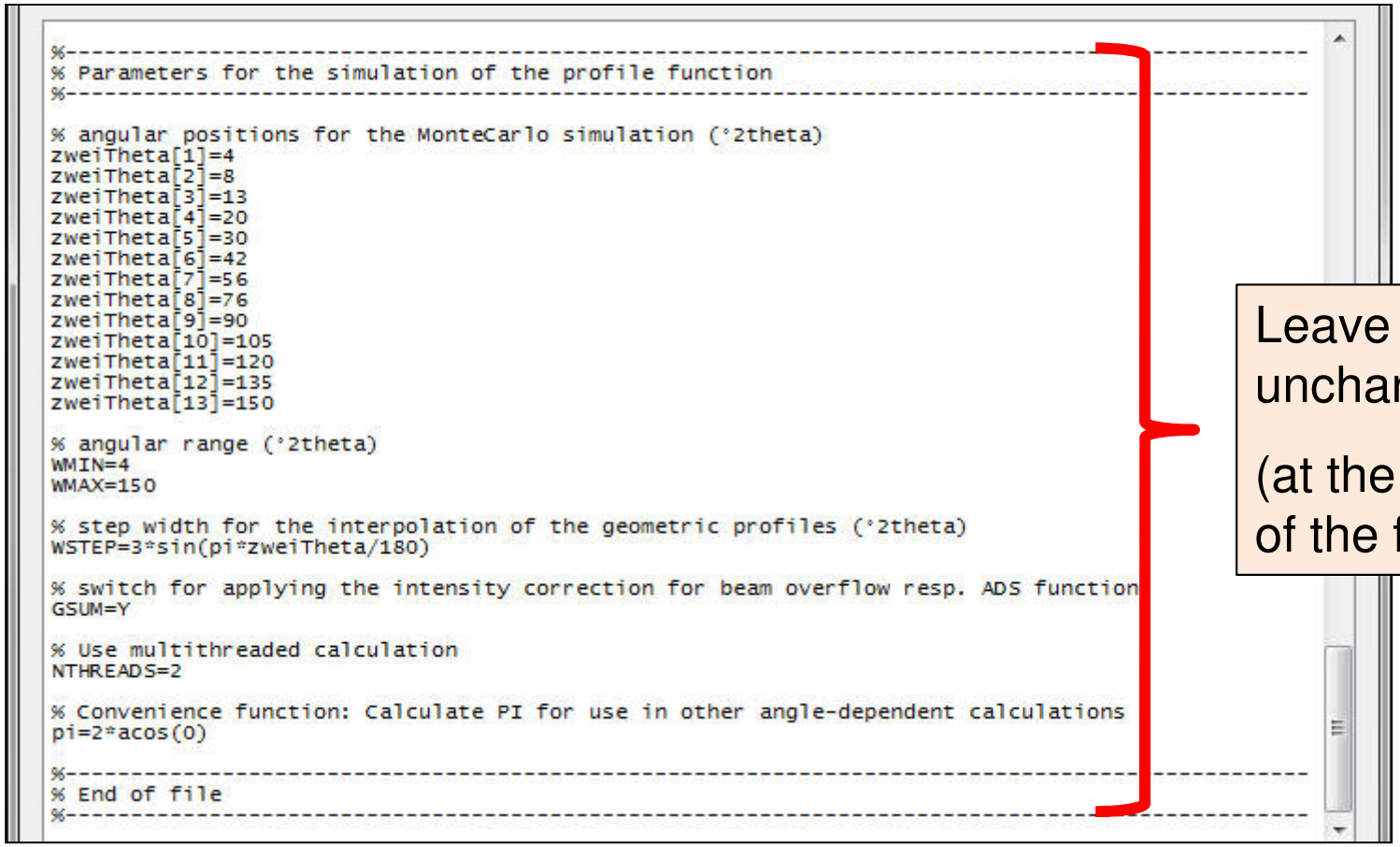


Editing Instrument Files



- Go through the file line by line
- Change values to match your configuration
- Verify **ALL** values

Editing Instrument Files

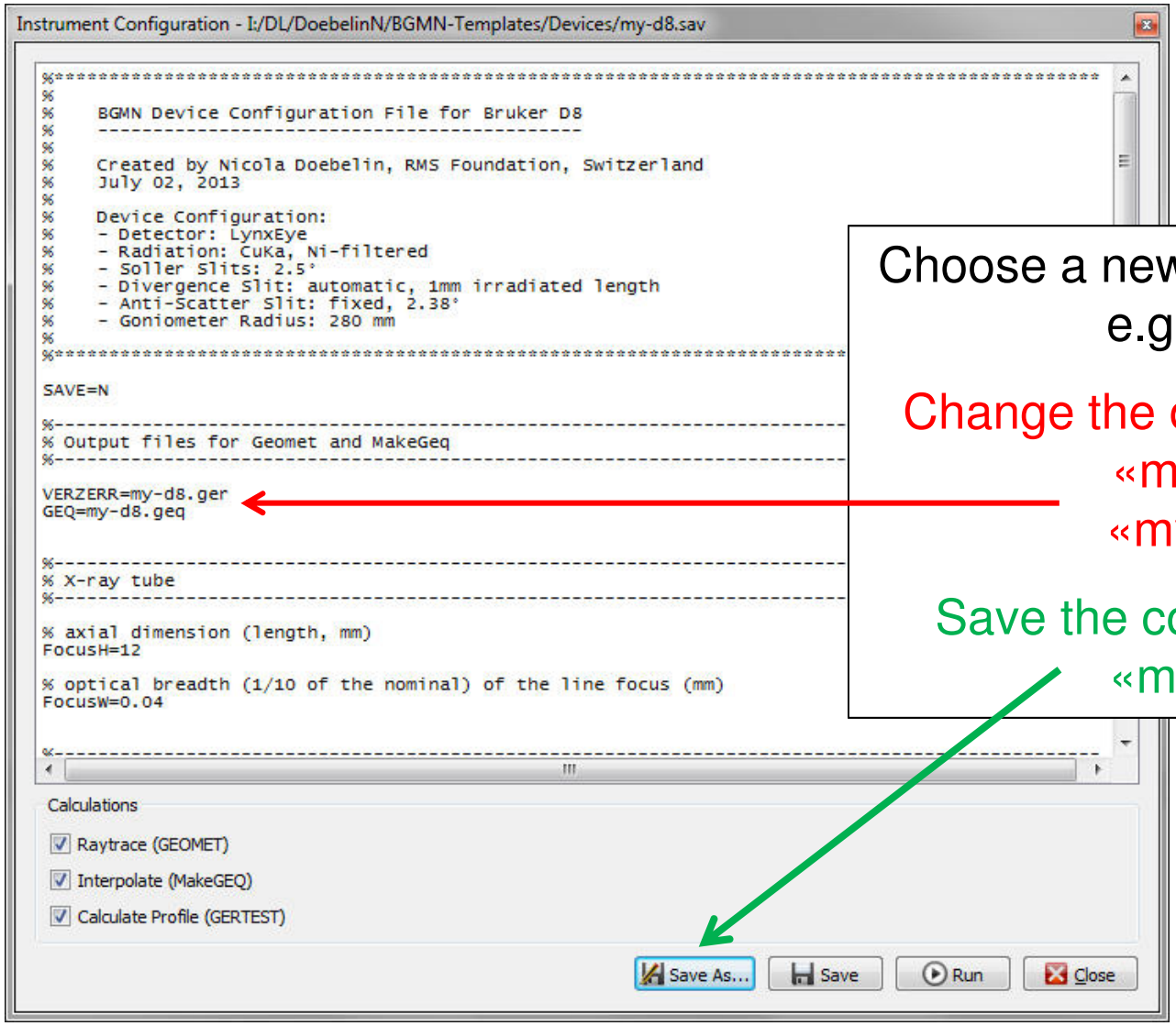


```
%--------------------------------------------------------------------------------
% Parameters for the simulation of the profile function
%--------------------------------------------------------------------------------

% angular positions for the MonteCarlo simulation (°2theta)
zweiTheta[1]=4
zweiTheta[2]=8
zweiTheta[3]=13
zweiTheta[4]=20
zweiTheta[5]=30
zweiTheta[6]=42
zweiTheta[7]=56
zweiTheta[8]=76
zweiTheta[9]=90
zweiTheta[10]=105
zweiTheta[11]=120
zweiTheta[12]=135
zweiTheta[13]=150

% angular range (°2theta)
WMIN=4
WMAX=150

% step width for the interpolation of the geometric profiles (°2theta)
WSTEP=3*sin(pi*zweiTheta/180)

% switch for applying the intensity correction for beam overflow resp. ADS function
GSUM=Y

% Use multithreaded calculation
NTHREADS=2

% Convenience function: Calculate PI for use in other angle-dependent calculations
pi=2*acos(0)

%--------------------------------------------------------------------------------
% End of file
%--------------------------------------------------------------------------------
```

Leave this block unchanged

(at the very end of the file)

Editing Instrument Files

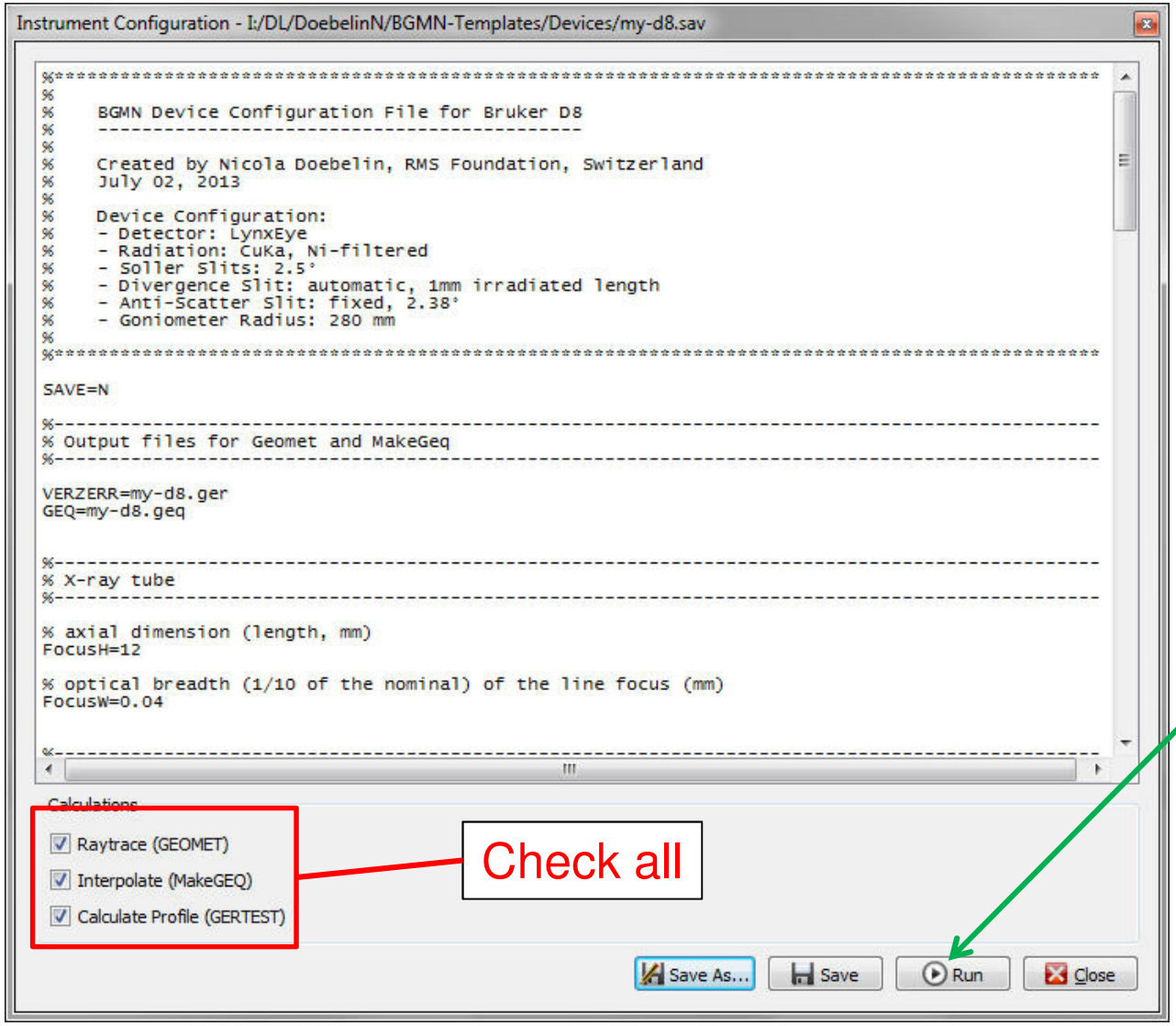


Choose a new configuration name
e.g. «my-d8»

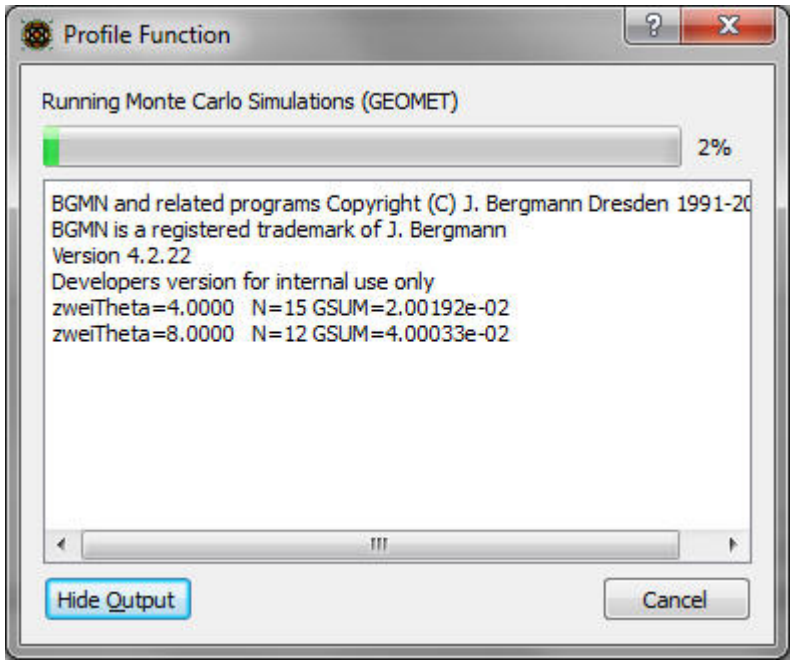
Change the output file names to
«my-d8.ger»
«my-d8.geq»

Save the configuration file as
«my-d8.sav»

Computing Peak Profile

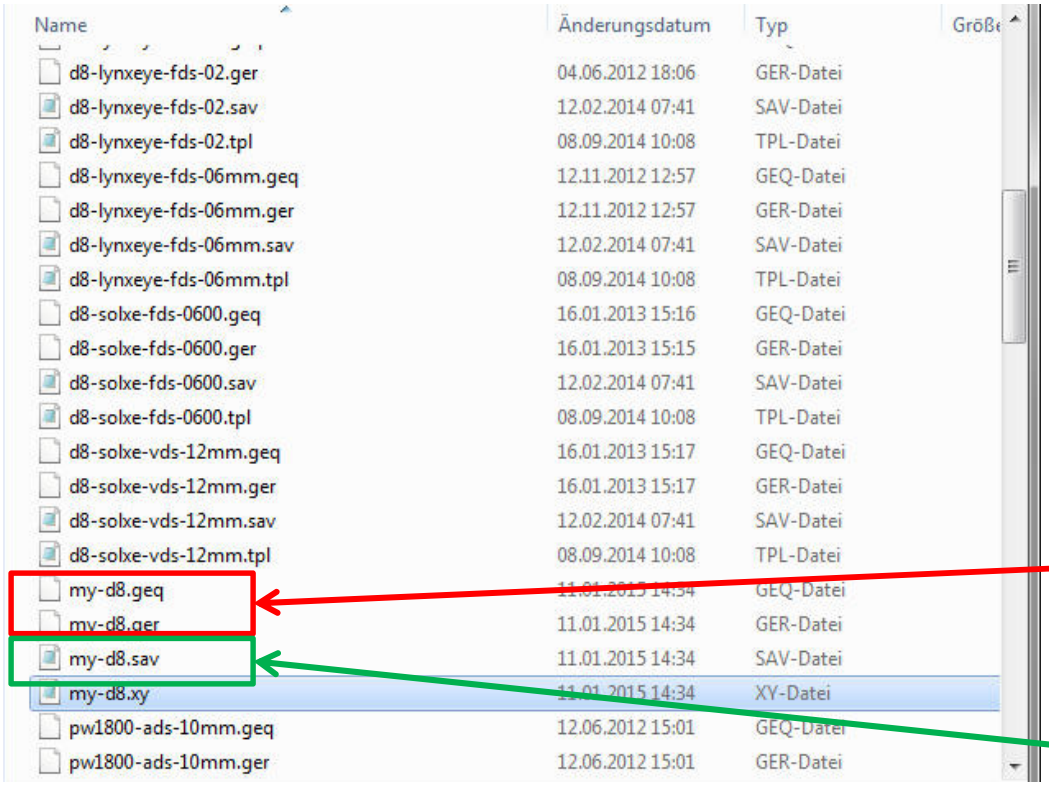


Computing Peak Profile



Computation may take several minutes

Computing Peak Profile



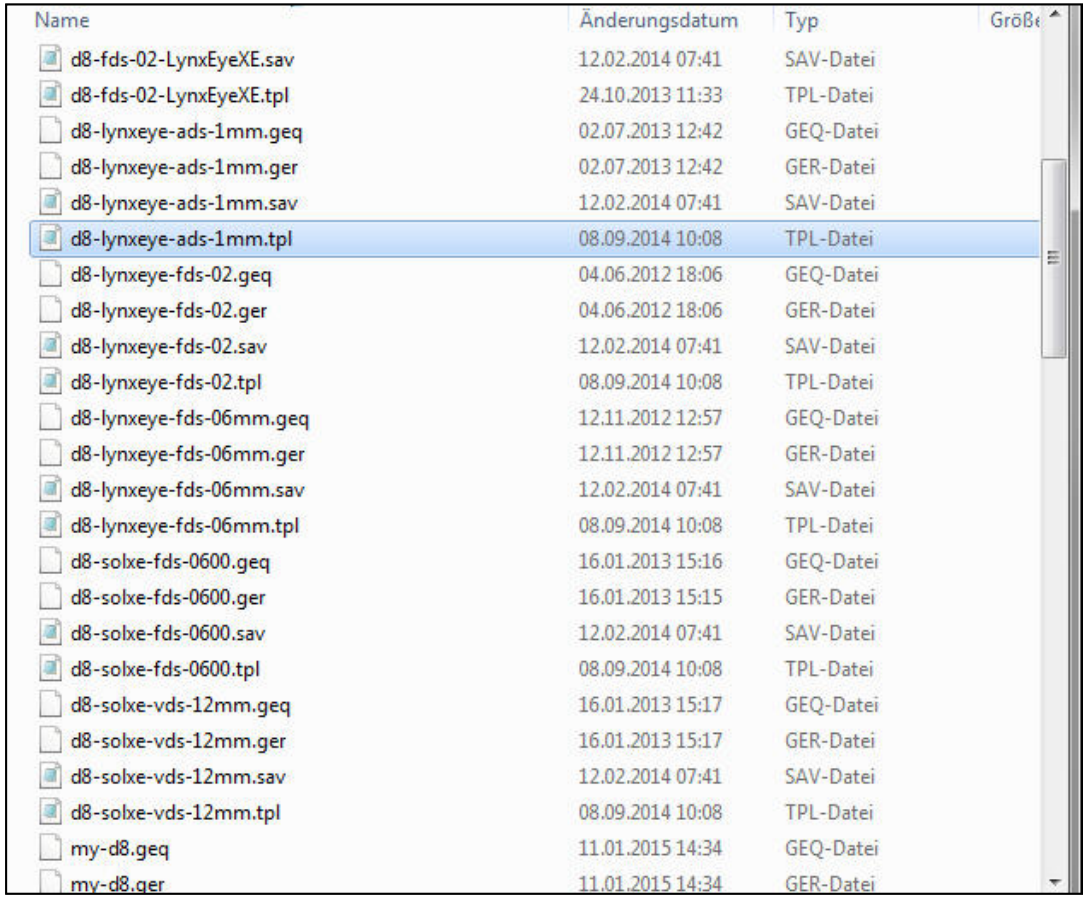
Name	Änderungsdatum	Typ	Größe
d8-lynxeye-fds-02.ger	04.06.2012 18:06	GER-Datei	
d8-lynxeye-fds-02.sav	12.02.2014 07:41	SAV-Datei	
d8-lynxeye-fds-02.tpl	08.09.2014 10:08	TPL-Datei	
d8-lynxeye-fds-06mm.geq	12.11.2012 12:57	GEQ-Datei	
d8-lynxeye-fds-06mm.ger	12.11.2012 12:57	GER-Datei	
d8-lynxeye-fds-06mm.sav	12.02.2014 07:41	SAV-Datei	
d8-lynxeye-fds-06mm.tpl	08.09.2014 10:08	TPL-Datei	
d8-solxe-fds-0600.geq	16.01.2013 15:16	GEQ-Datei	
d8-solxe-fds-0600.ger	16.01.2013 15:15	GER-Datei	
d8-solxe-fds-0600.sav	12.02.2014 07:41	SAV-Datei	
d8-solxe-fds-0600.tpl	08.09.2014 10:08	TPL-Datei	
d8-solxe-vds-12mm.geq	16.01.2013 15:17	GEQ-Datei	
d8-solxe-vds-12mm.ger	16.01.2013 15:17	GER-Datei	
d8-solxe-vds-12mm.sav	12.02.2014 07:41	SAV-Datei	
d8-solxe-vds-12mm.tpl	08.09.2014 10:08	TPL-Datei	
my-d8.geq	11.01.2015 14:34	GEQ-Datei	
my-d8.ger	11.01.2015 14:34	GER-Datei	
my-d8.sav	11.01.2015 14:34	SAV-Datei	
my-d8.xy	11.01.2015 14:34	XY-Datei	
pw1800-ads-10mm.geq	12.06.2012 15:01	GEQ-Datei	
pw1800-ads-10mm.ger	12.06.2012 15:01	GER-Datei	

Computed peak profile

Instrument description

Template SAV file (*.tpl)

Template file for *.sav control file:



Name	Änderungsdatum	Typ	Größe
d8-fds-02-LynxEyeXE.sav	12.02.2014 07:41	SAV-Datei	
d8-fds-02-LynxEyeXE.tpl	24.10.2013 11:33	TPL-Datei	
d8-lynxeye-ads-1mm.geq	02.07.2013 12:42	GEQ-Datei	
d8-lynxeye-ads-1mm.ger	02.07.2013 12:42	GER-Datei	
d8-lynxeye-ads-1mm.sav	12.02.2014 07:41	SAV-Datei	
d8-lynxeye-ads-1mm.tpl	08.09.2014 10:08	TPL-Datei	
d8-lynxeye-fds-02.geq	04.06.2012 18:06	GEQ-Datei	
d8-lynxeye-fds-02.ger	04.06.2012 18:06	GER-Datei	
d8-lynxeye-fds-02.sav	12.02.2014 07:41	SAV-Datei	
d8-lynxeye-fds-02.tpl	08.09.2014 10:08	TPL-Datei	
d8-lynxeye-fds-06mm.geq	12.11.2012 12:57	GEQ-Datei	
d8-lynxeye-fds-06mm.ger	12.11.2012 12:57	GER-Datei	
d8-lynxeye-fds-06mm.sav	12.02.2014 07:41	SAV-Datei	
d8-lynxeye-fds-06mm.tpl	08.09.2014 10:08	TPL-Datei	
d8-solxe-fds-0600.geq	16.01.2013 15:16	GEQ-Datei	
d8-solxe-fds-0600.ger	16.01.2013 15:15	GER-Datei	
d8-solxe-fds-0600.sav	12.02.2014 07:41	SAV-Datei	
d8-solxe-fds-0600.tpl	08.09.2014 10:08	TPL-Datei	
d8-solxe-vds-12mm.geq	16.01.2013 15:17	GEQ-Datei	
d8-solxe-vds-12mm.ger	16.01.2013 15:17	GER-Datei	
d8-solxe-vds-12mm.sav	12.02.2014 07:41	SAV-Datei	
d8-solxe-vds-12mm.tpl	08.09.2014 10:08	TPL-Datei	
my-d8.geq	11.01.2015 14:34	GEQ-Datei	
my-d8.ger	11.01.2015 14:34	GER-Datei	

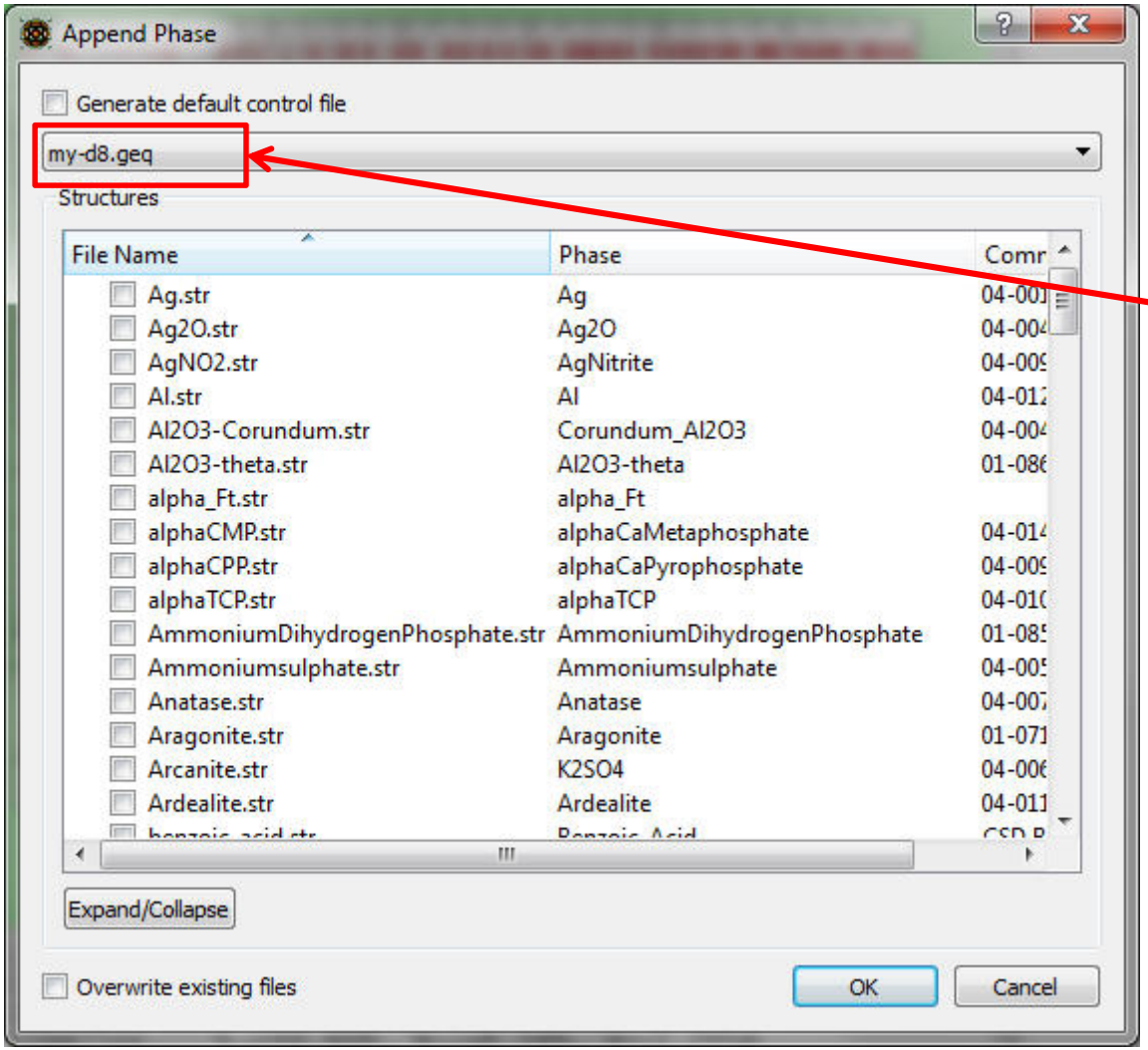
Copy

«d8-lynxeye-ads-1mm.tpl»

to

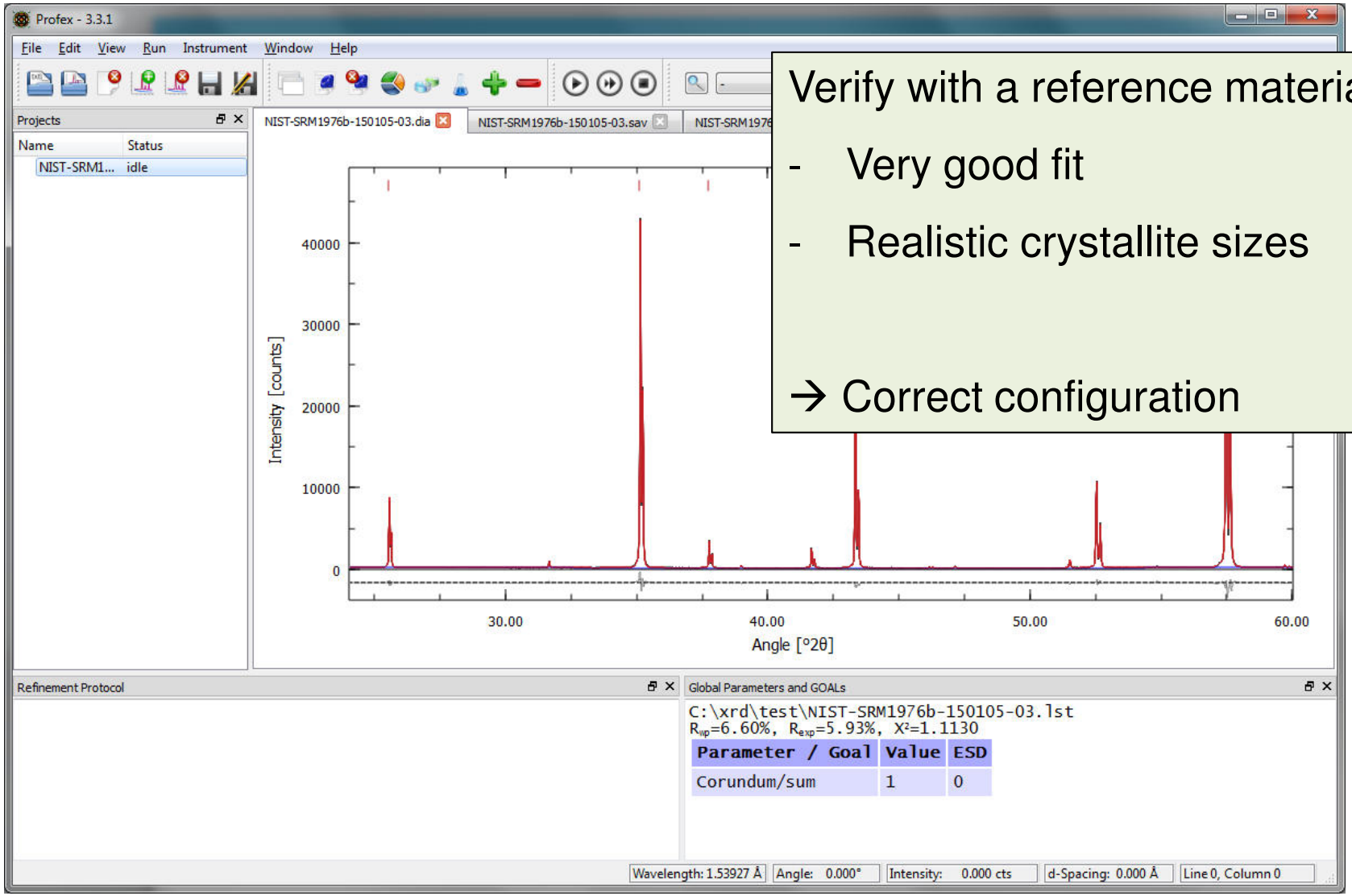
«my-d8.tpl»

Append Phase



In «Add Phase» dialog (+)

Verification



Verify with a reference material:

- Very good fit ✓
- Realistic crystallite sizes ✓

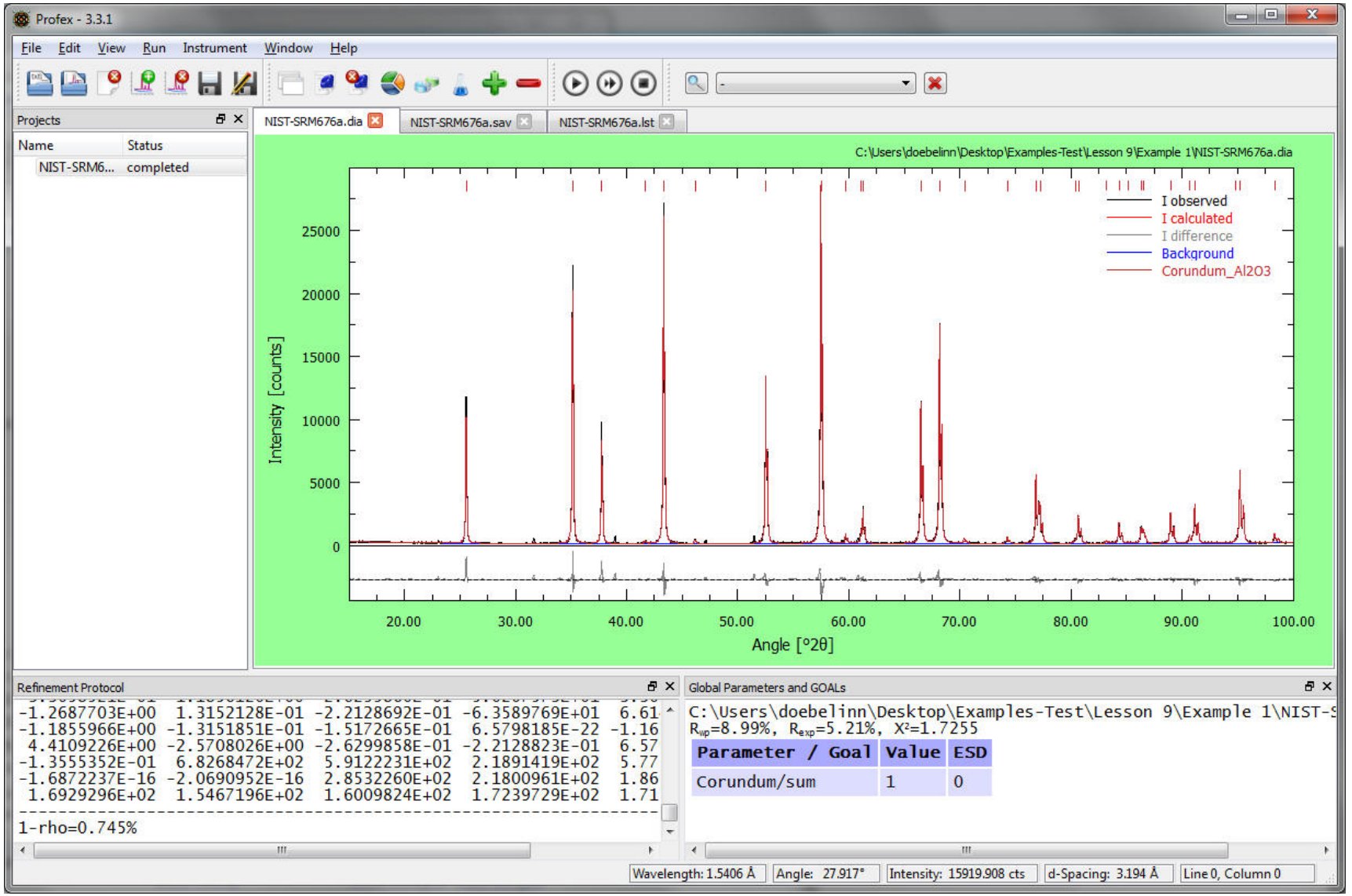
→ Correct configuration ✓

Lesson 9: Example 1

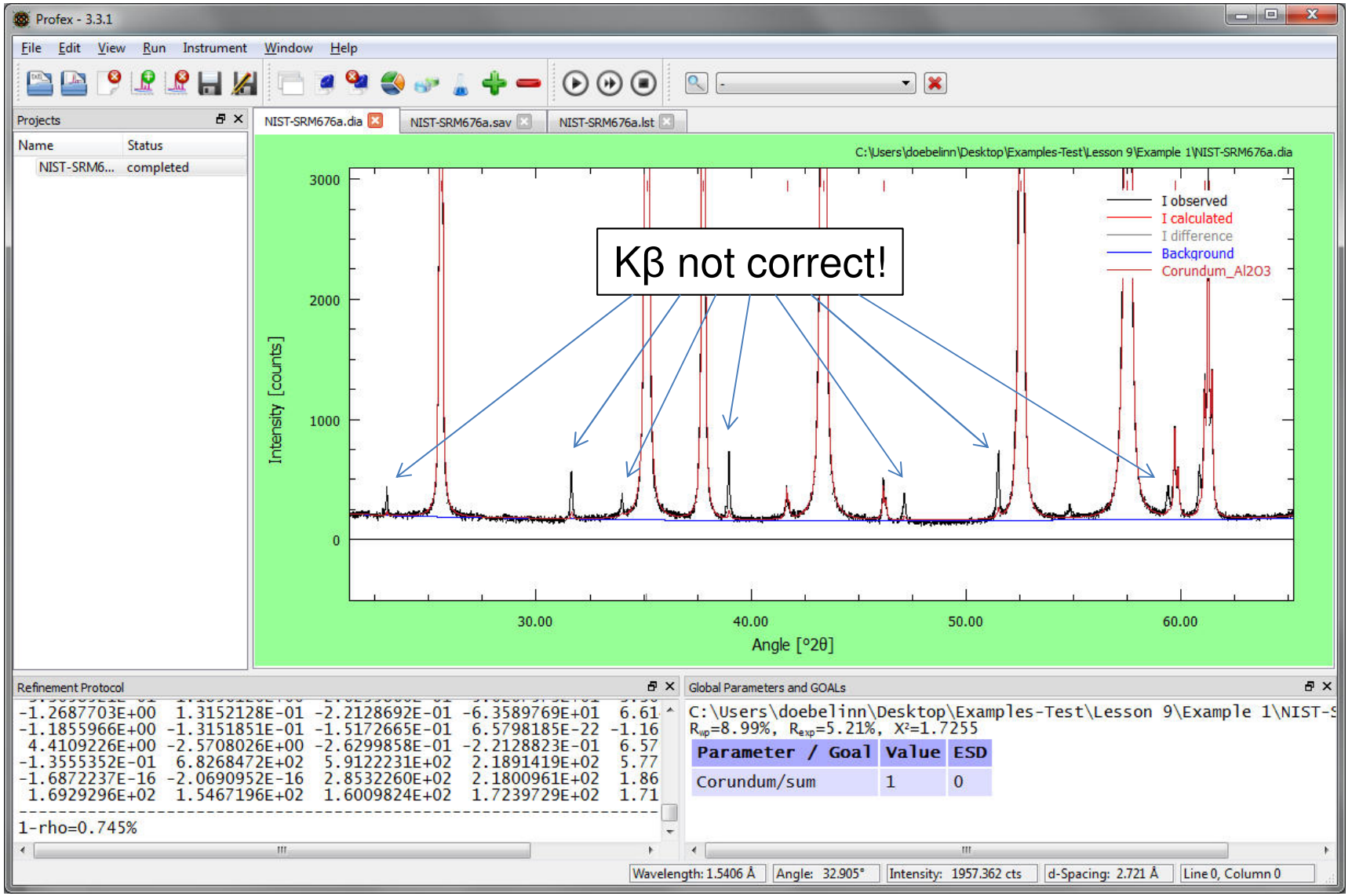
Instrument:	Bruker D8 Advance
Geometry:	Reflection
Goniometer Radius:	350 mm
X-ray Tube:	CuKa, Target Size 12 x 0.4 mm
Divergence Slit:	Automatic, 15 mm irr. length Distance to sample 250 mm
Soller Slits:	2.5° in prim. and sec. beam
Beam Mask:	Width 10.5 mm Distance from sample 300 mm
Sample Diameter:	25 mm
Anti-Scatter Slit:	9mm Distance to sample 260 mm
Detector Slit:	Not installed
Detector:	LynxEye XE Array height 14.4 mm Height of one strip 0.075 mm Array width 16.0 mm Number of channels 192
Beam Knife:	Not installed
Polarization:	None

1. Start from configuration «d8-lynxeye-ads-1mm.sav»
2. Modify according to
3. Save under a new name «d8-lesson9-example1.sav»
4. «Run» to compute peak profile
5. Copy template file «d8-lynxeye-ads-1mm.tpl» to «d8-lesson9-example1.tpl»
6. Verify configuration with scan «SRM-676a.raw»

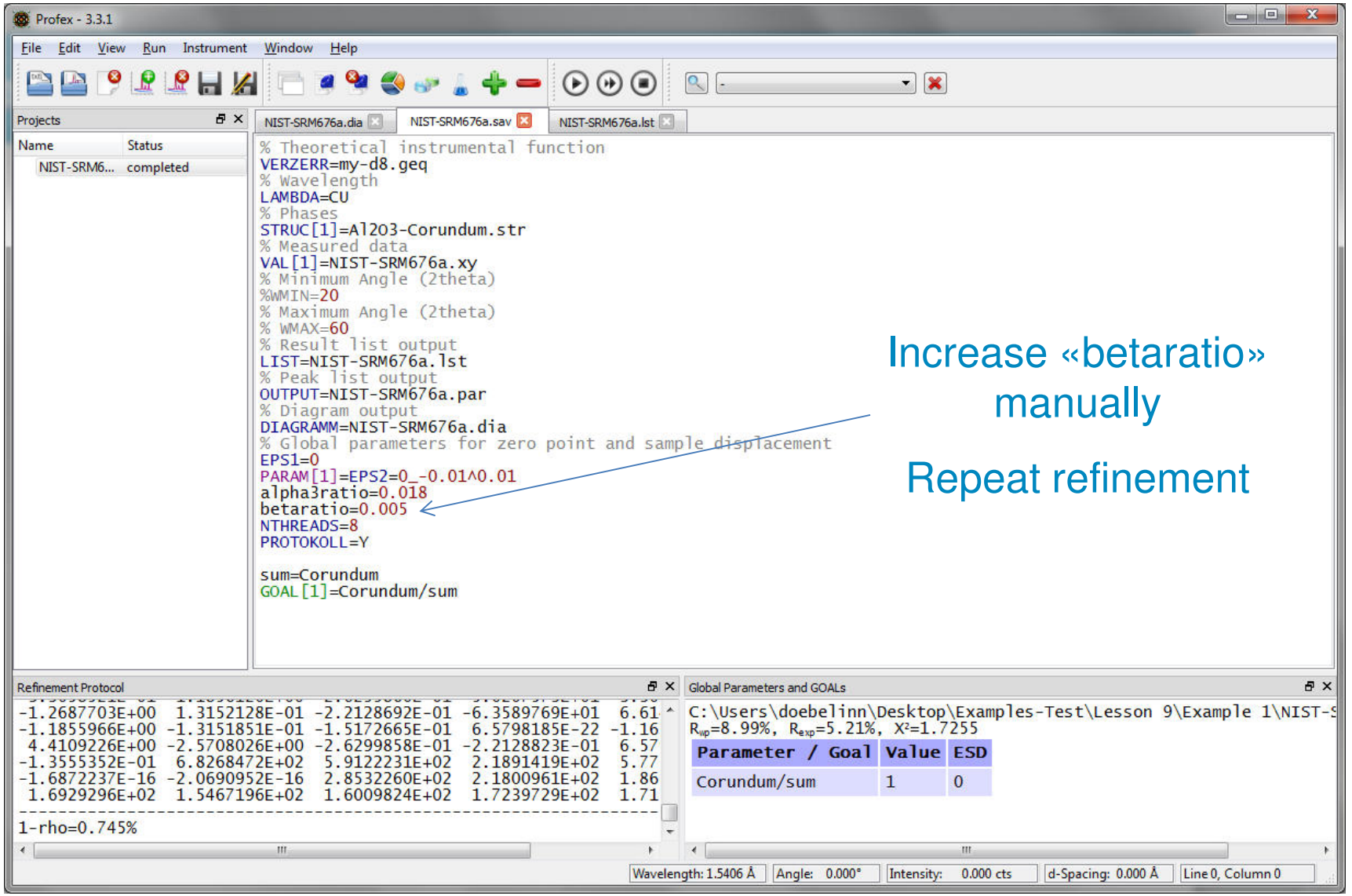
Lesson 9: Example 1



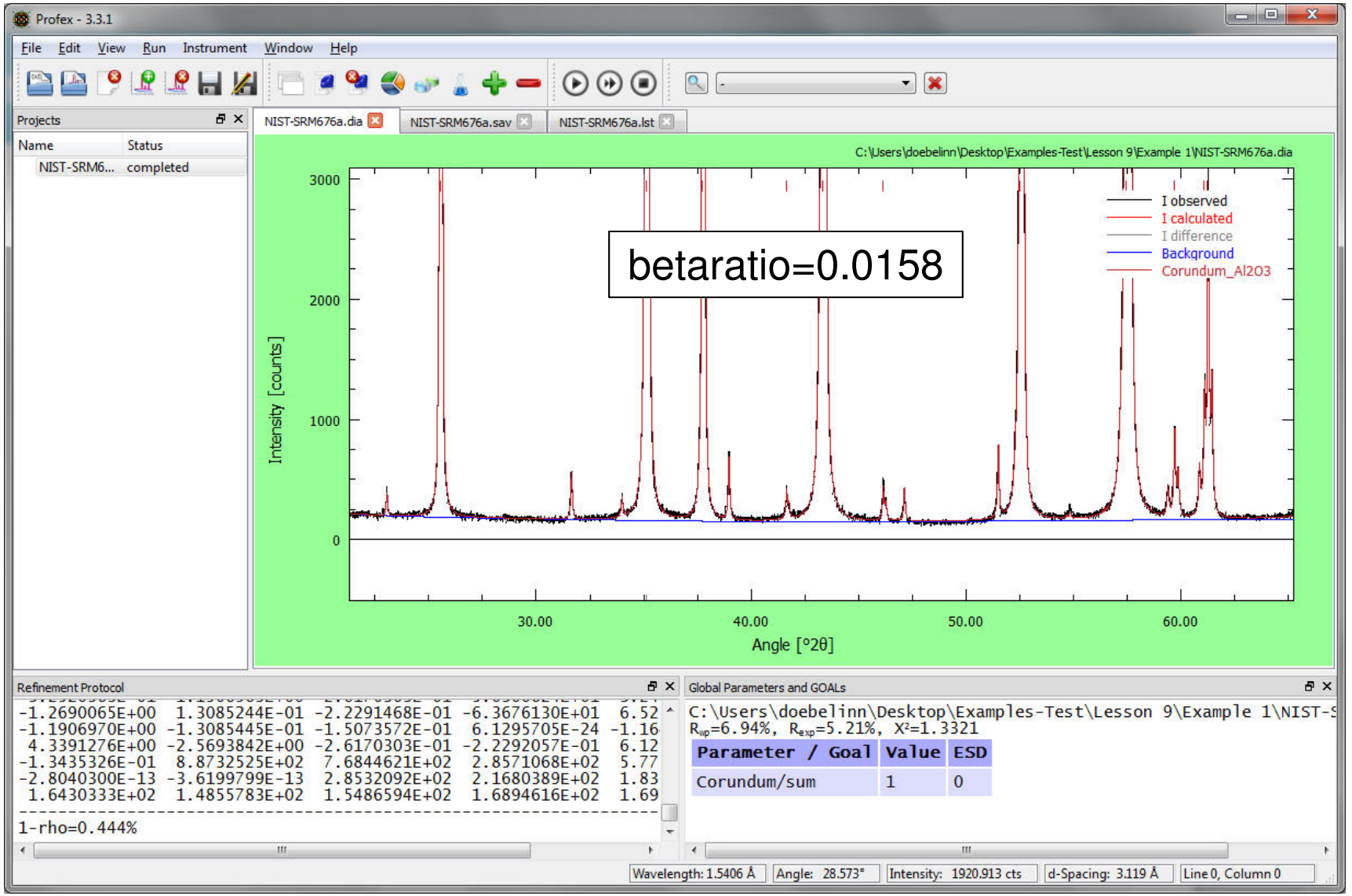
Lesson 9: Example 1



Lesson 9: Example 1

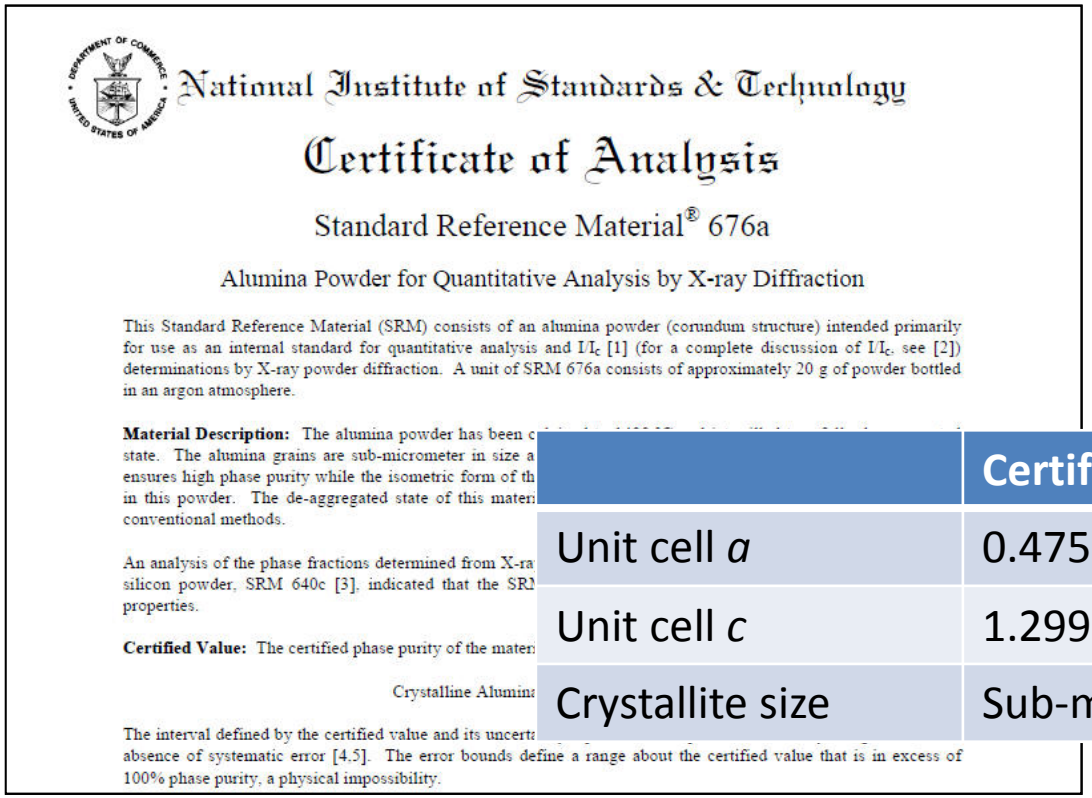


Lesson 9: Example 1



Lesson 9: Example 1

- Verify refined unit cell dimensions and crystallite size with SRM certificate



National Institute of Standards & Technology

Certificate of Analysis

Standard Reference Material® 676a

Alumina Powder for Quantitative Analysis by X-ray Diffraction

This Standard Reference Material (SRM) consists of an alumina powder (corundum structure) intended primarily for use as an internal standard for quantitative analysis and I/I_c [1] (for a complete discussion of I/I_c, see [2]) determinations by X-ray powder diffraction. A unit of SRM 676a consists of approximately 20 g of powder bottled in an argon atmosphere.

Material Description: The alumina powder has been c
state. The alumina grains are sub-micrometer in size a
ensures high phase purity while the isometric form of th
in this powder. The de-aggregated state of this materi
conventional methods.

An analysis of the phase fractions determined from X-ra
silicon powder, SRM 640c [3], indicated that the SR
properties.

Certified Value: The certified phase purity of the mater

Crystalline Alumina

The interval defined by the certified value and its uncerta
absence of systematic error [4.5]. The error bounds define a range about the certified value that is in excess of 100% phase purity, a physical impossibility.

	Certified	Refined
Unit cell *a*	0.475936 nm	0.476021 nm
Unit cell *c*	1.29923 nm	1.299485 nm
Crystallite size	Sub-micron	131 nm

Lesson 9: Example 1

- Write betaratio=0.0158 to «d8-lesson9-example1.tpl»