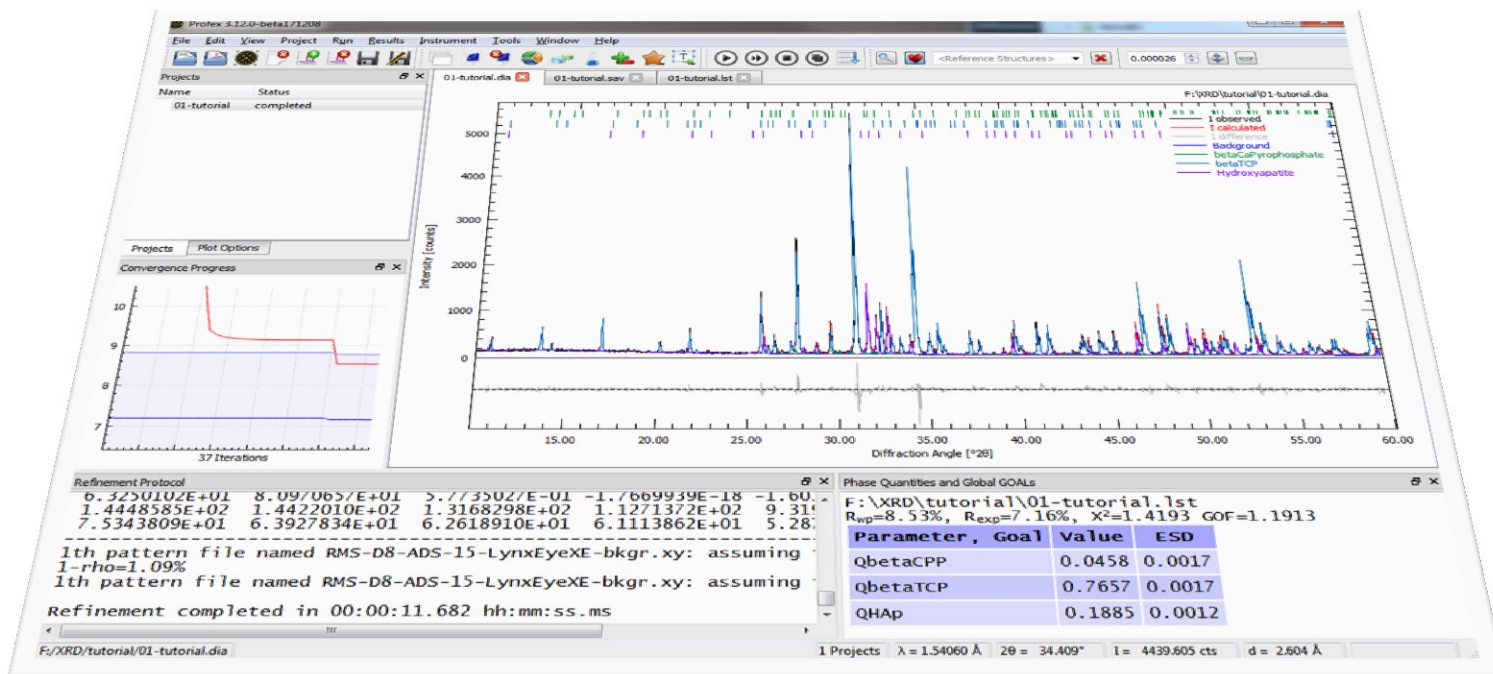


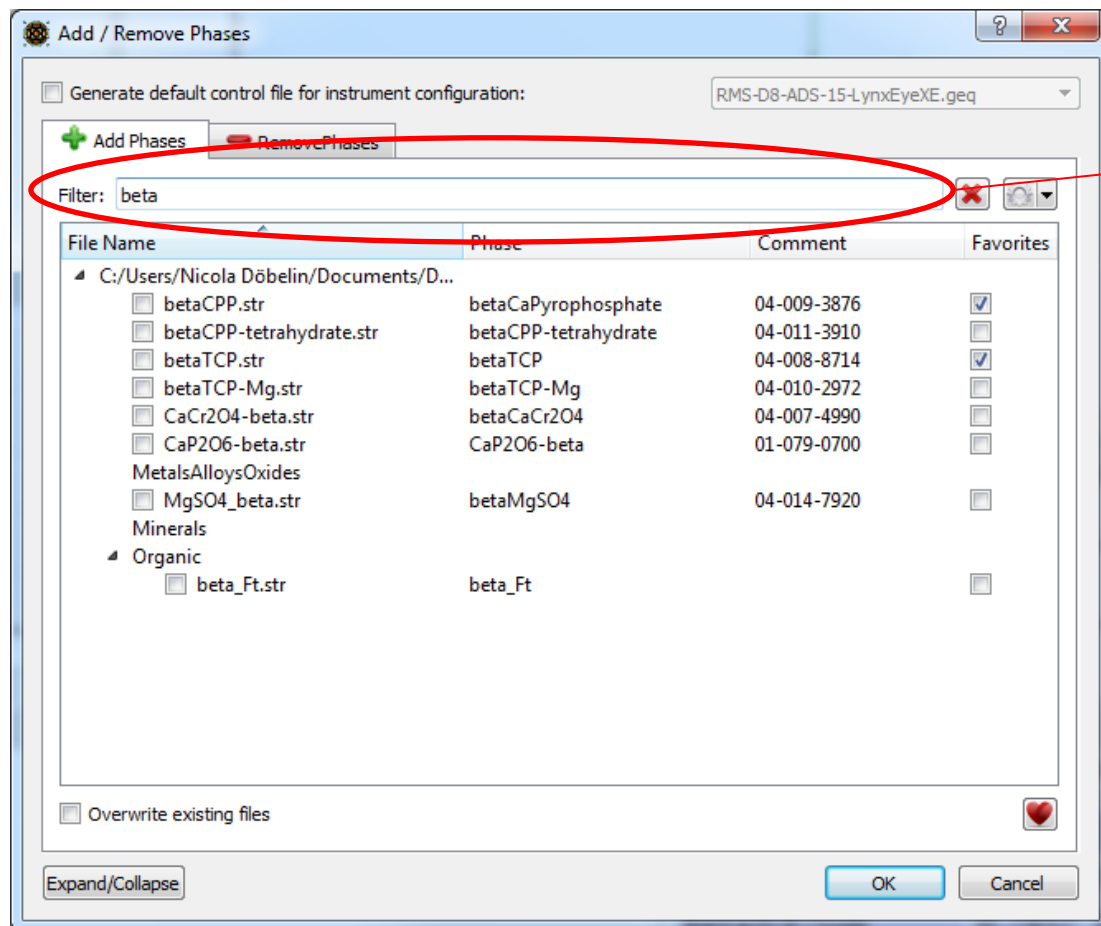
# PROFEX

OPEN SOURCE XRD AND RIETVELD REFINEMENT

## New features in Profex 3.12



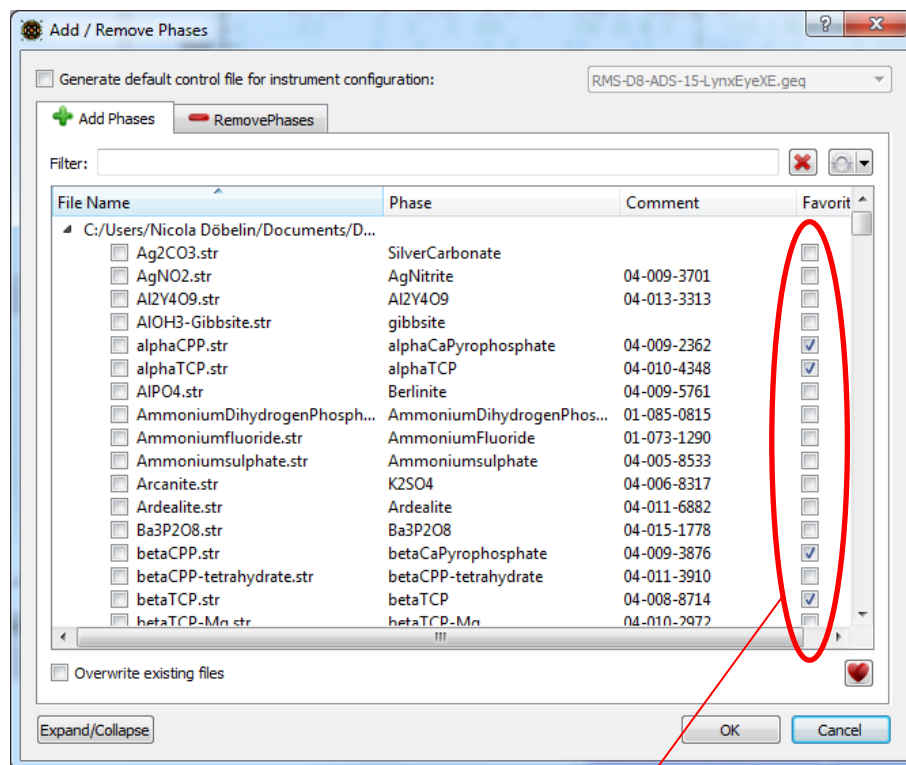
## Filter phases in Add/Remove Phase dialog



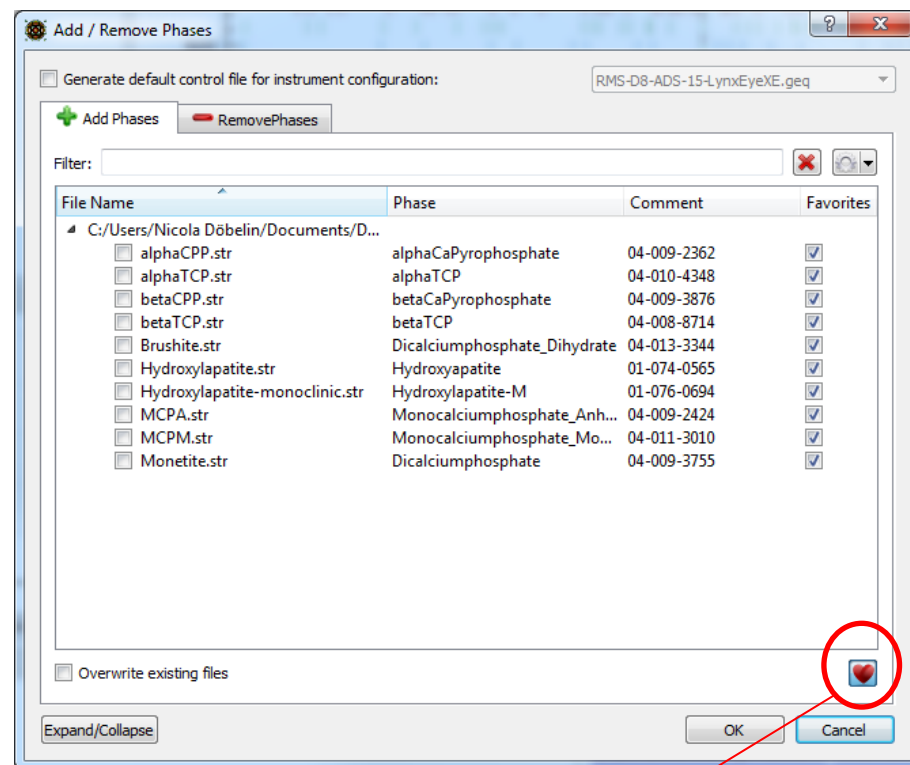
1. Enter a filter string

2. The structure list will be filtered instantly

## Favorite phases in Add/Remove Phase dialog

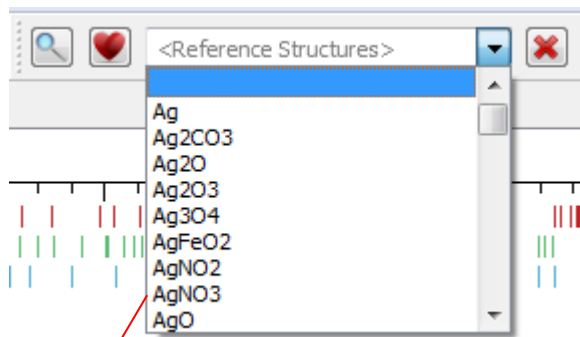


1. Select favorite phases

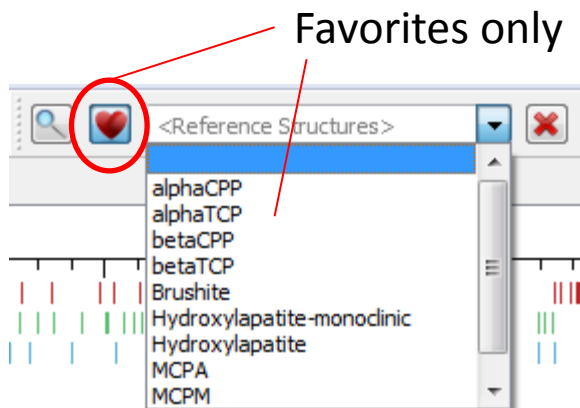


2. Only display favorites

The same favorites also apply to the reference structure list

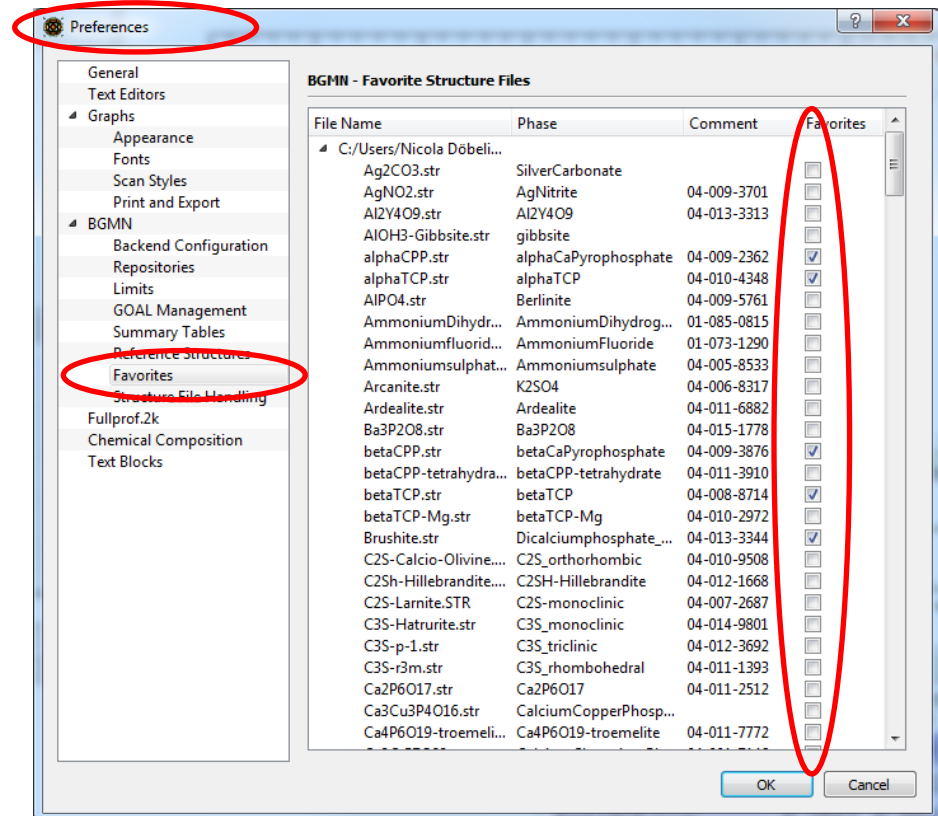


All phases



Favorites only

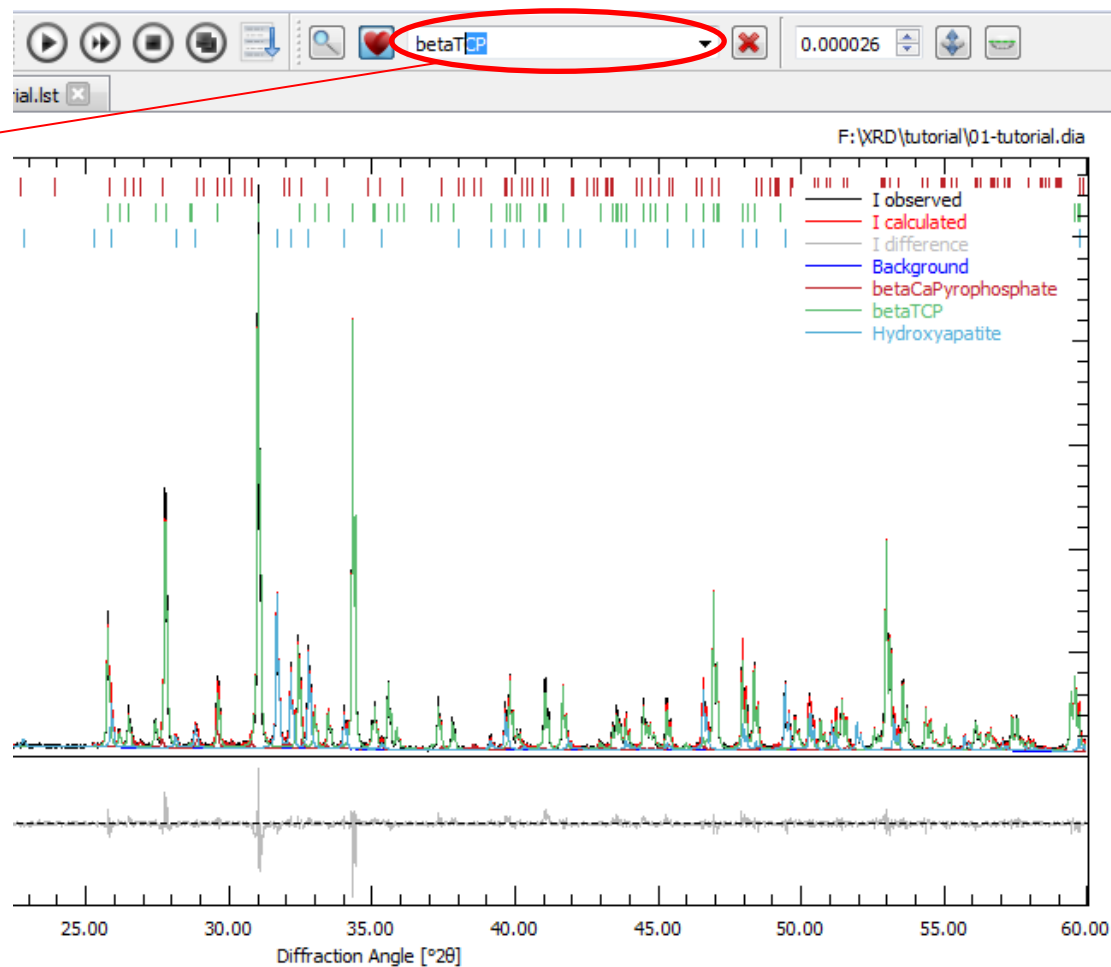
Configure favorites in preferences dialog





## Auto-completion in reference structure menu

1. Start typing in the menu box
2. Auto-completion will propose a reference phase
3. Press <<Enter>> to accept



## New Tool: Calculate Absorption Coefficients

From refinement  
project

User-specified

**Absorption Coefficient**

**Phase Parameters**

Phase: betaCaPyrophosphate  
 Empirical formula: CA16 O56 P16  
 Density [g/cm<sup>3</sup>]: 3.1270  
 Phase quantity: 0.0458

**Sample Parameters**

Wavelength: CuKα1  
 Attenuation [%]: 99.00  
 Packing density [%]: 100.00  
 Incident angle [°]: 30.00

**Absorption**

Phase MAC [cm<sup>2</sup>/g]: 77.10324  
 Phase LAC [cm<sup>-1</sup>]: 241.10183  
 Sample MAC [cm<sup>2</sup>/g]: 85.48405  
 Sample LAC [cm<sup>-1</sup>]: 263.58281  
 Path length [μm]: 174.7144  
 Layer thickness [μm]: 87.3572

MAC: Mass absorption coefficient  
 LAC: Linear absorption coefficient

Phase	Formula	Density [g/cm <sup>3</sup> ]	Quantity	Phase MAC [cm <sup>2</sup> /g]	Phase LAC [cm <sup>-1</sup> ]
betaCaPyrophosphate	CA16 O56 P16	3.1270	0.0458	77.10324	241.10183
betaTCP	CA63 O168 P42	3.0680	0.7657	85.72296	262.99805
Hydroxyapatite	CA10 H2 O26 P6	3.1360	0.1885	86.54988	271.42041

Close

Abs. Coefficient...

... For phases

... For the sample

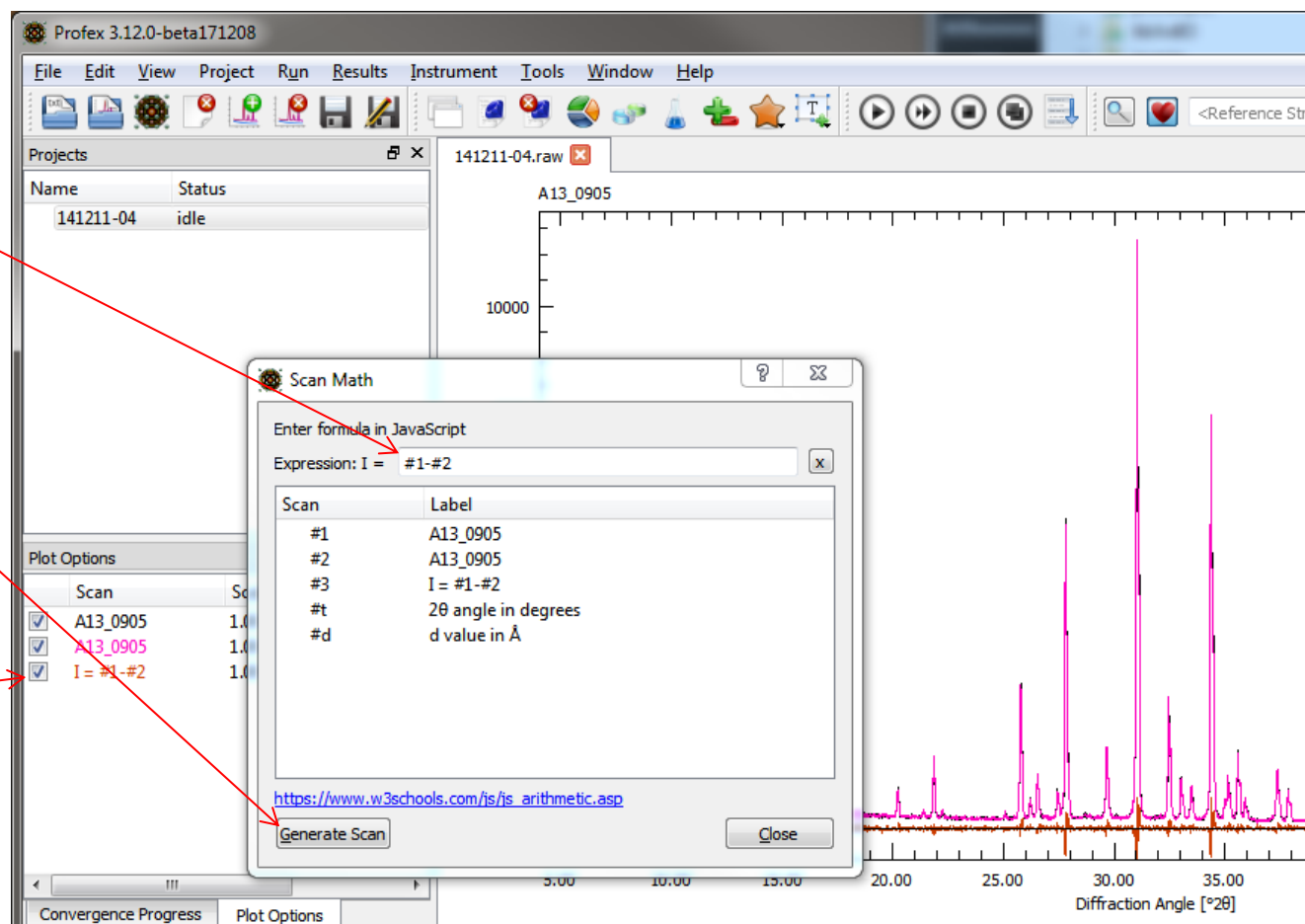
Penetration depth

## New Tool: Mathematical operations on Scans

1. Enter mathematical expression

2. Generate scan

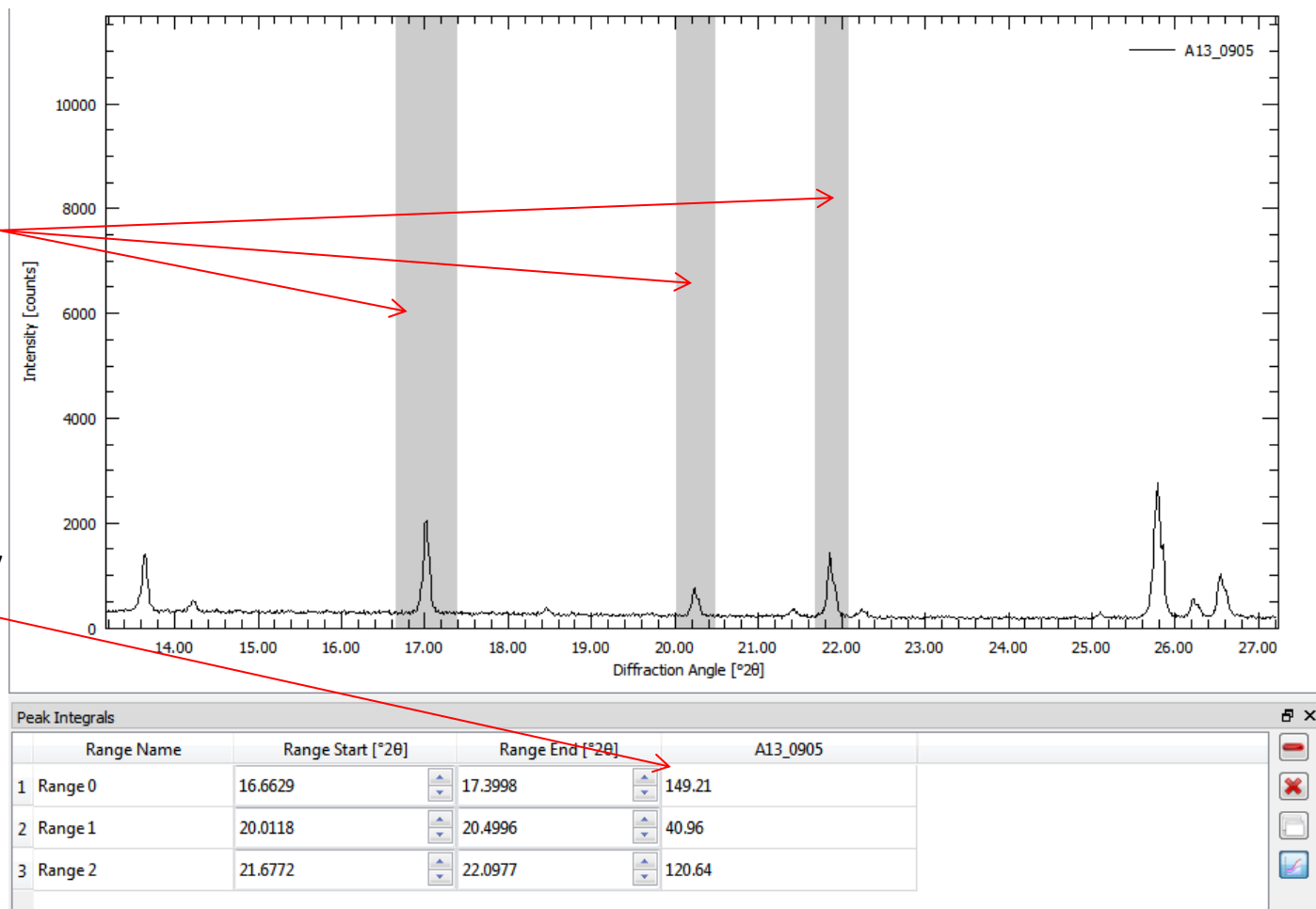
3. New scan will be appended to the project



## New Tool: Integrate peak intensities

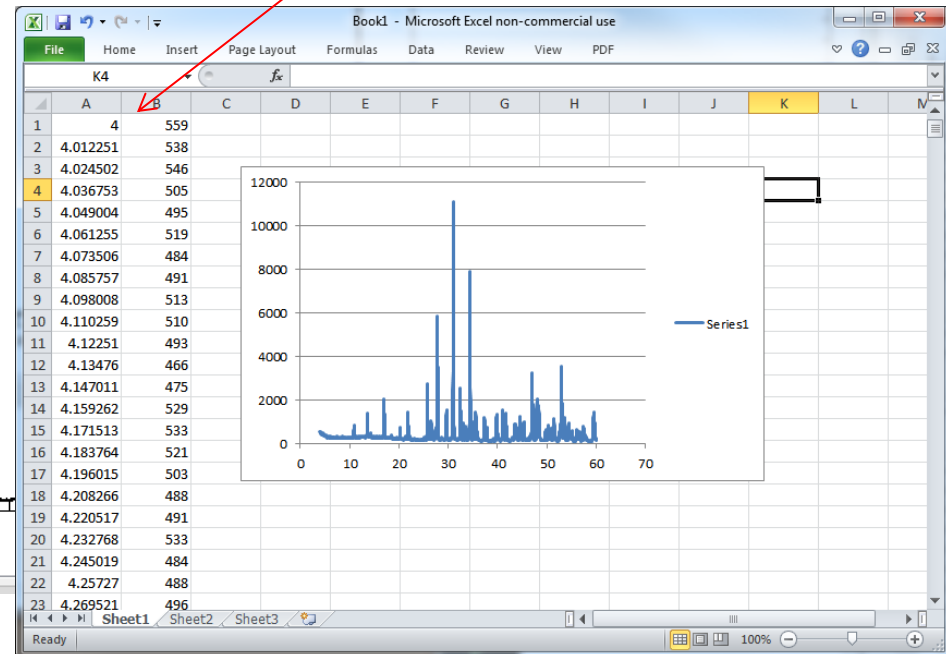
1. Use <<Shift>>  
+ left mouse button  
to define integration  
ranges

2. Integrated intensity  
will be calculated



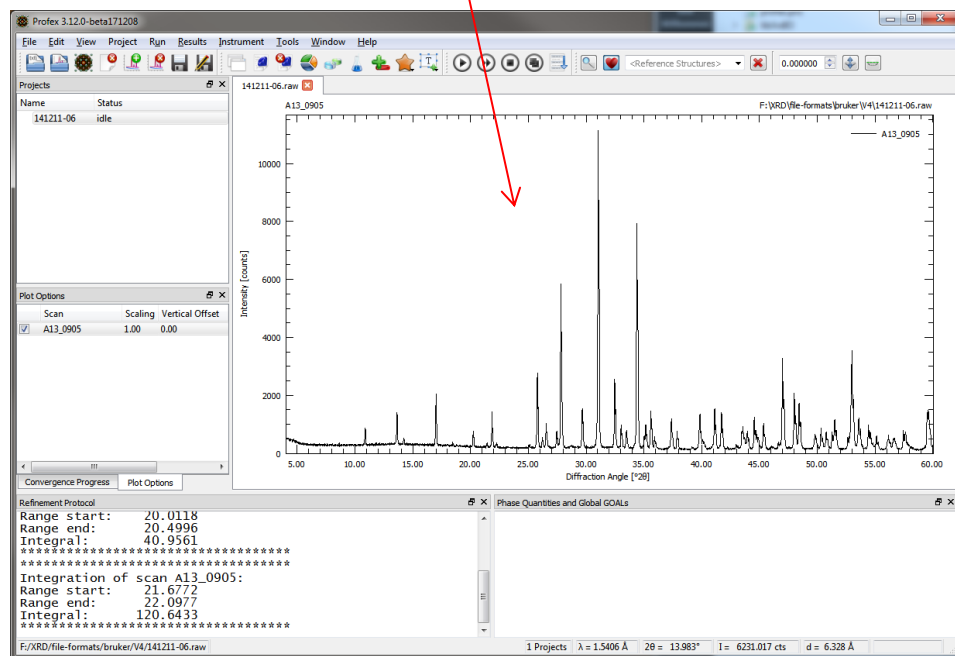


## 1. Right mouse button in Plot Options list

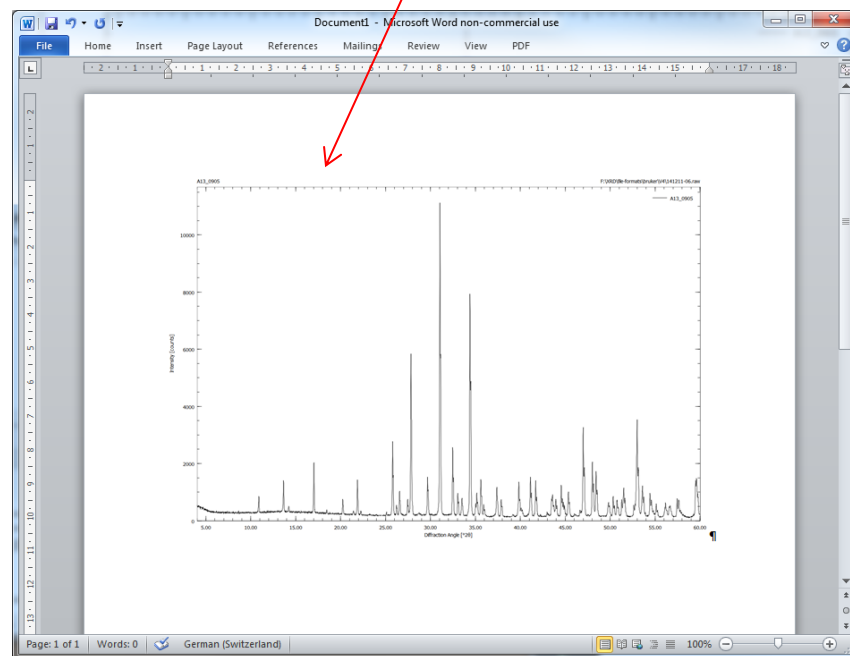


## Copy scan pixel image to clipboard

1. <<Ctrl + C>> on graph display



2. <<Ctrl + V>> in other application



## New syntax for quantification GOALS (optional)

```

RU=10
% Measured data
VAL[1]=01-tutorial.xy
% Minimum Angle (2theta)
WMIN=10
% Maximum Angle (2theta)
% WMAX=60
% Result list output
LIST=01-tutorial.lst
% Peak list output
OUTPUT=01-tutorial.par
% Diagram output
DIAGRAMM=01-tutorial.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=0.005
NTHREADS=8
PROTOKOLL=Y
SAVE=N

sum=betaCPP+betaTCP+HAp
QbetaCPP=betaCPP/sum
QbetaTCP=betaTCP/sum
QHAp=HAp/sum

GOAL [1]=QbetaCPP
GOAL [2]=QbetaTCP
GOAL [3]=QHAp
    
```

Parameter	Goal	Value	ESD
QbetaCPP		0.0458	0.0017
QbetaTCP		0.7657	0.0017
QHAp		0.1885	0.0012

Phase Quantities and Global GOALS

F:\XRD\tutorial\01-tutorial.lst  
R<sub>wp</sub>=8.53%, R<sub>exp</sub>=7.16%, X<sup>2</sup>=1.4193 GOF

08-ADS-15-LynxEyeXE-bkgr.xy: assuming  
08-ADS-15-LynxEyeXE-bkgr.xy: assuming  
00:11.682 hh:mm:ss.ms

1 Projects λ = 1.54060 Å 2θ = 0.000° I = 0.000 cts d

Preferences

- General
- Text Editors
- Graphs
  - Appearance
  - Fonts
  - Scan Styles
  - Print and Export
- BGMN
  - Backend Configuration
  - Repositories
  - Limits
  - GOAL Management**
  - Summary Tables
  - Reference Structures
  - Favorites
  - Structure File Handling
- Fullprof.2k
- Chemical Composition
- Text Blocks

**BGMN - GOAL Management**

☒ Manage Phase Quantification GOALS

GOAL syntax format: **Extended**

Relative Phase Quantity GOALS

GOAL name prefix: Q

Denominator variable: sum

Absolute Phase Quantity GOALS

GOAL name prefix: Qabs

Denominator variable: sumabs

☐ Also add GOALS for relative phase quantities

OK Cancel

Customize in  
preferences dialog  
(select old or new syntax)

# PROFEX

OPEN SOURCE XRD AND RIETVELD REFINEMENT

+ many bugfixes

