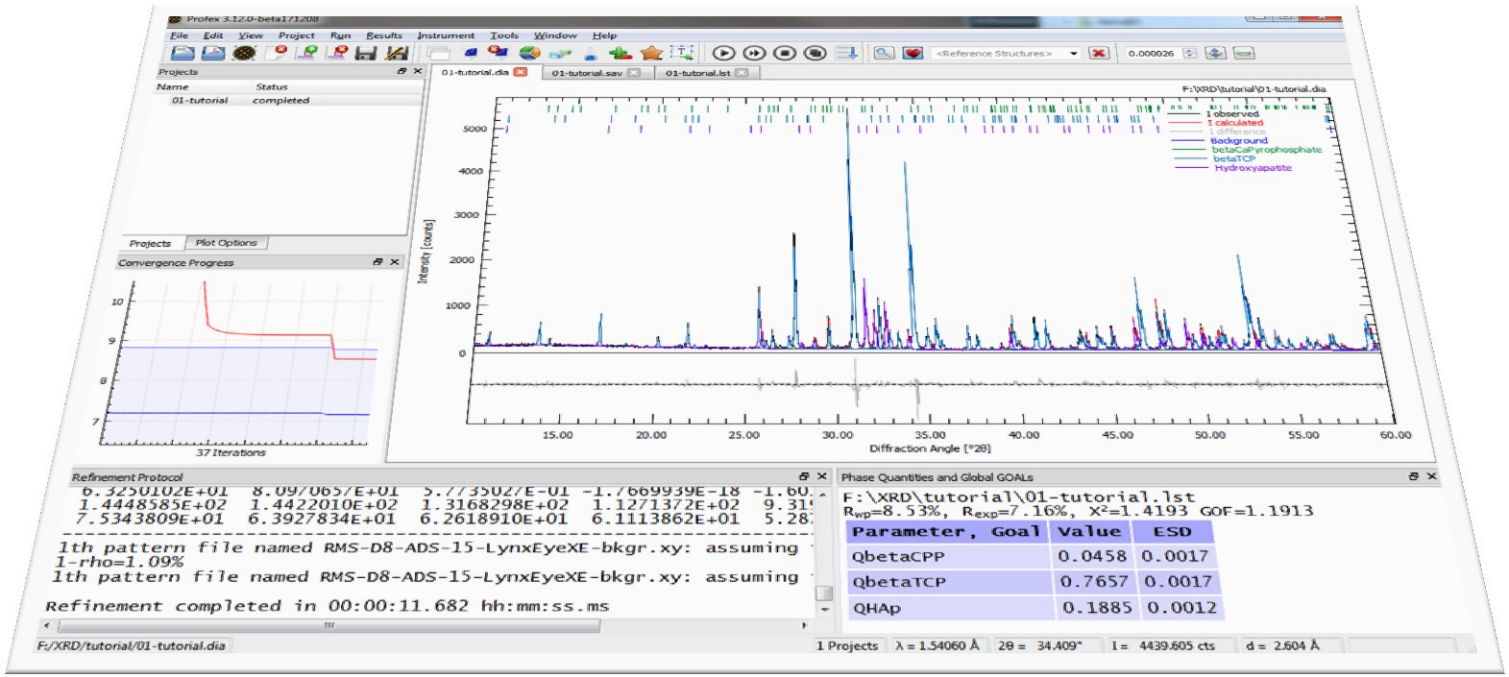
# PROFEX

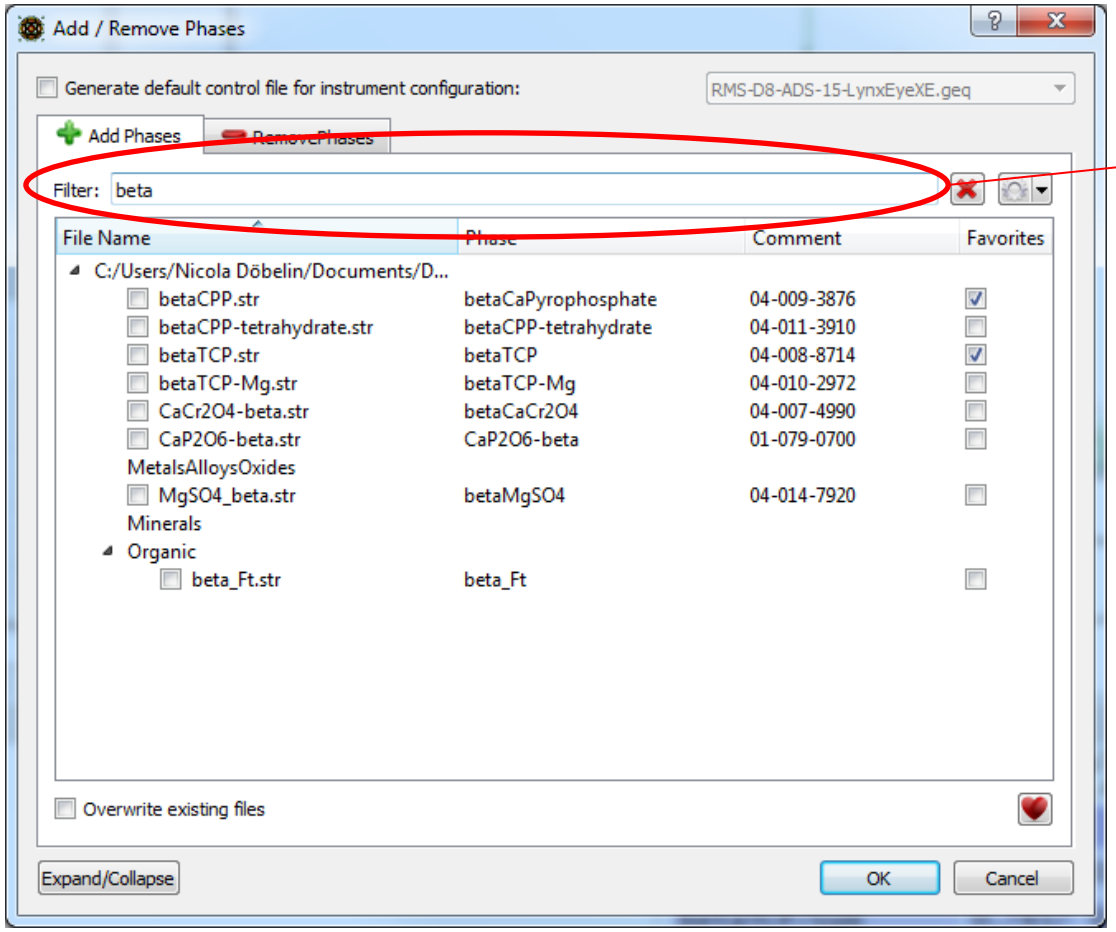
OPEN SOURCE XRD AND RIETVELD REFINEMENT

New features in Profex 3.12




December 2017, Nicola Döbelin

# Filter phases in Add/Remove Phase dialog




1. Enter a filter string

2. The structure list will be filtered instantly

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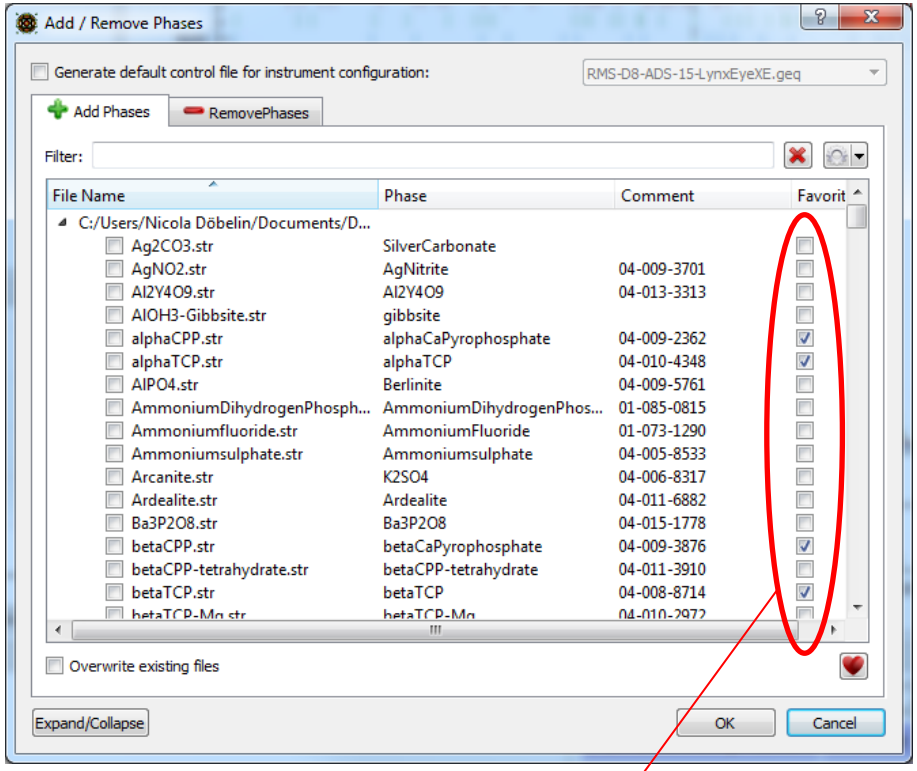
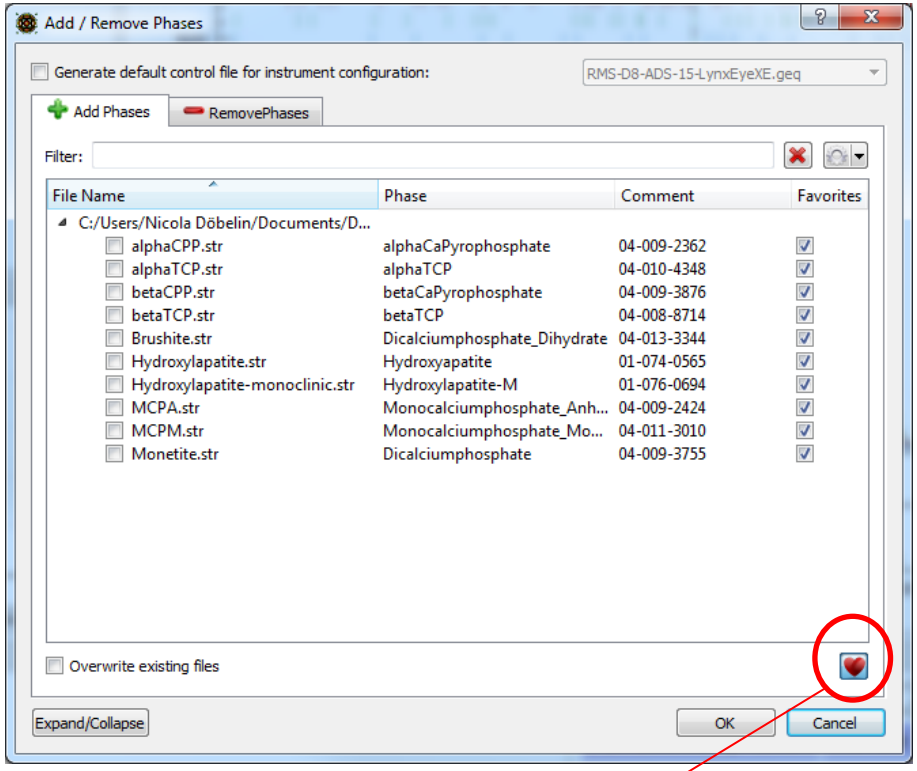
# Favorite phases in Add/Remove Phase dialog




1. Select favorite phases

2. Only display favorites

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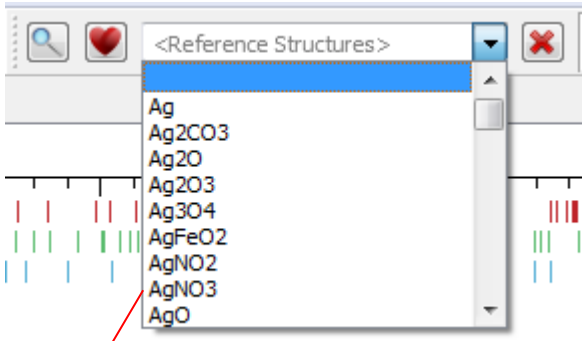
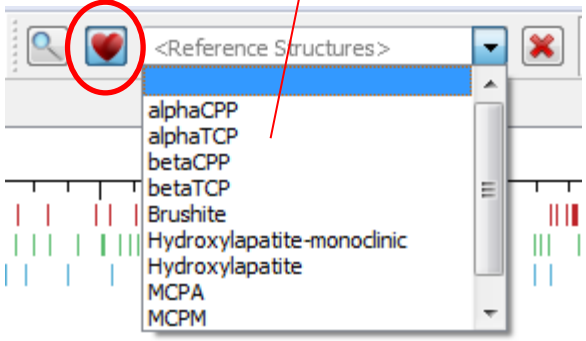
The same favorites also apply to the reference structure list

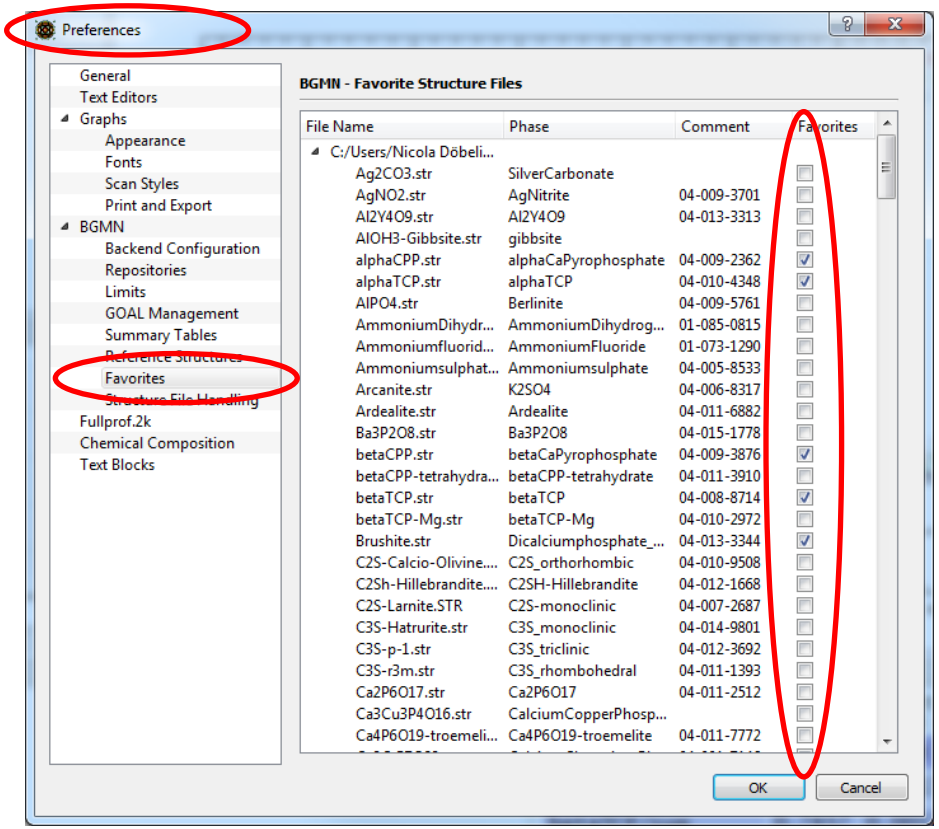



All phases

Favorites only




Configure favorites in preferences dialog

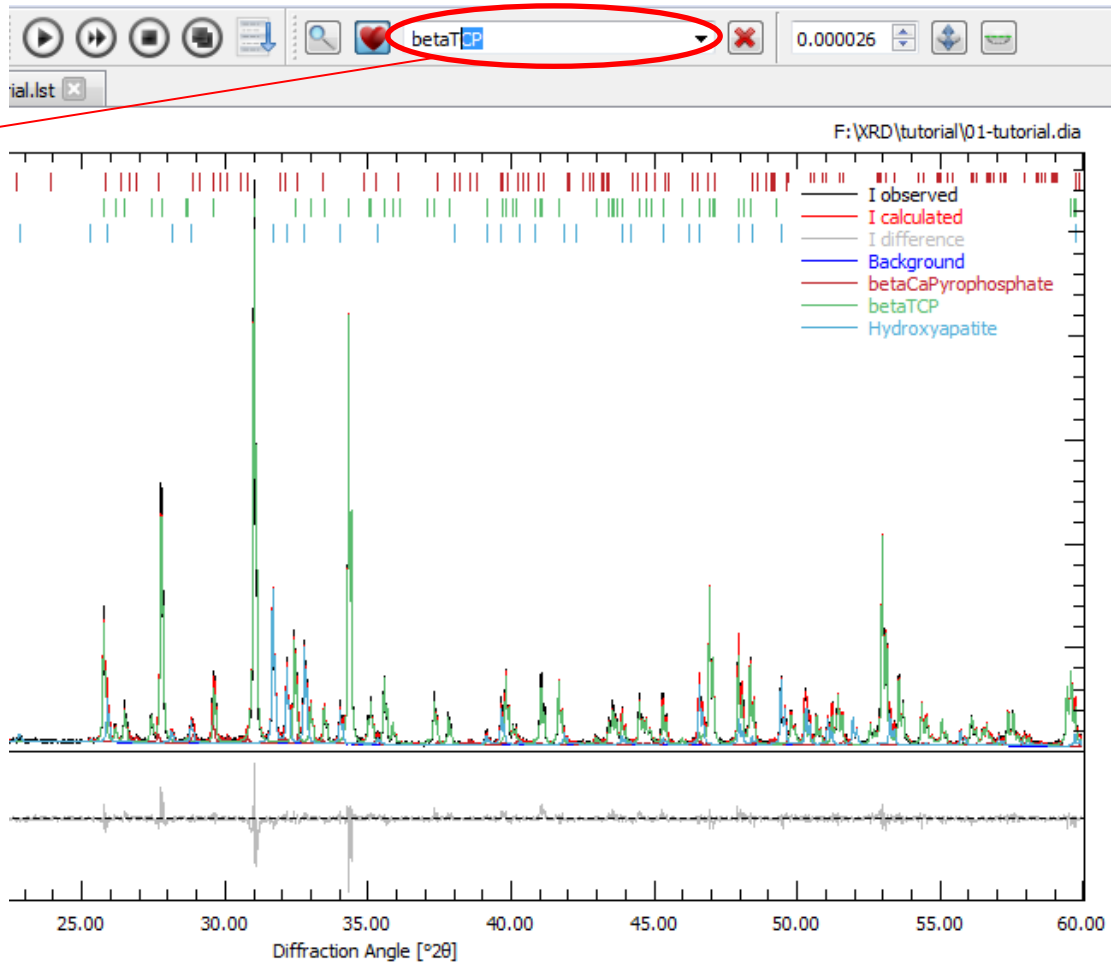


Auto-completion in reference structure menu

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

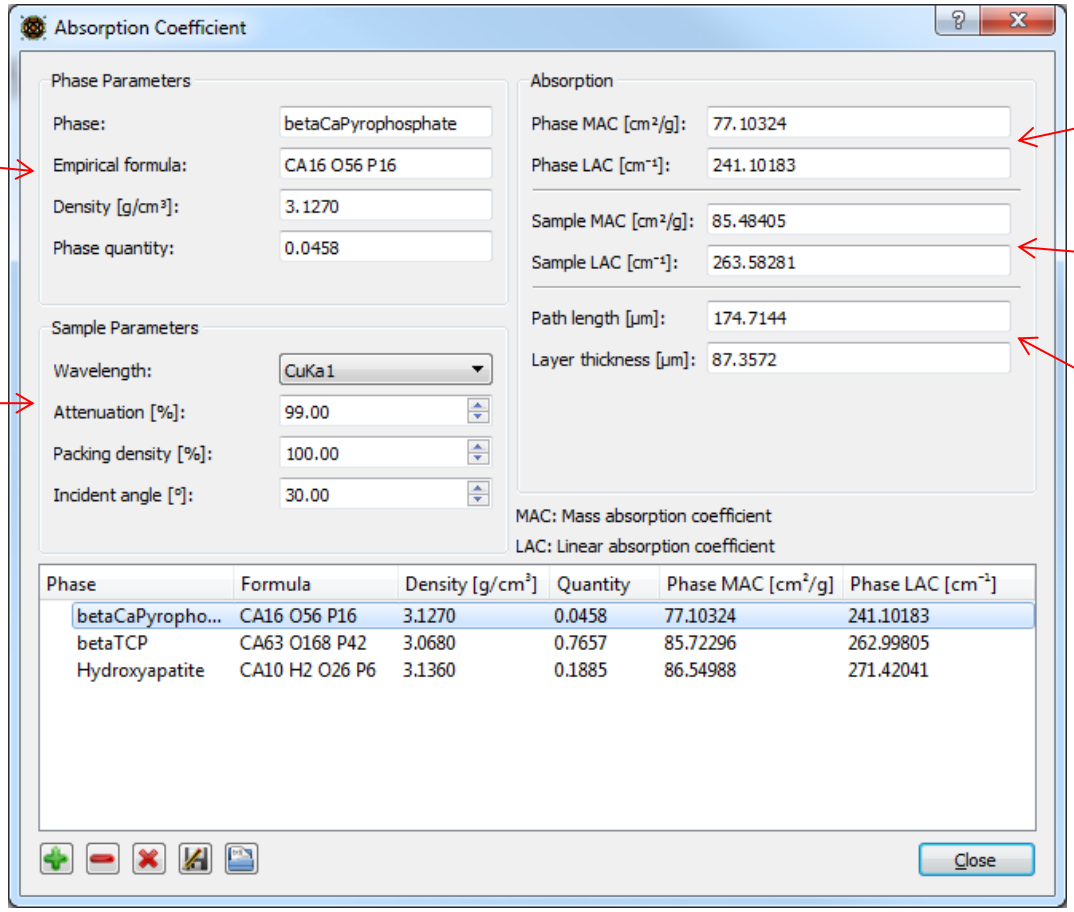
User-specified

Abs. Coefficient...

... For phases

... For the sample

Penetration depth



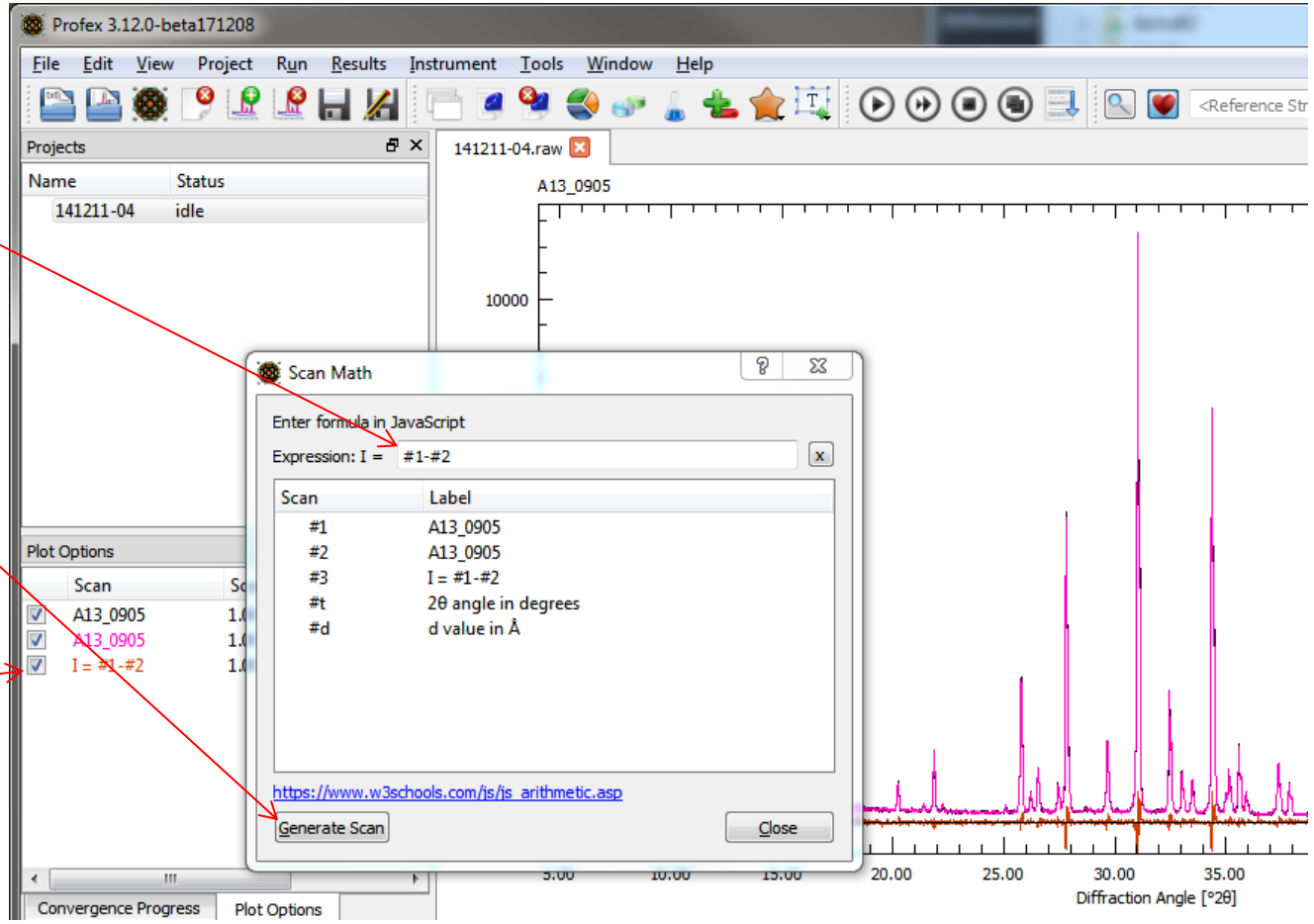

Tools → Calculate Absorption Coefficients...

# New Tool: Mathematical operations on Scans

1. Enter mathematical expression

2. Generate scan

3. New scan will be appended to the project

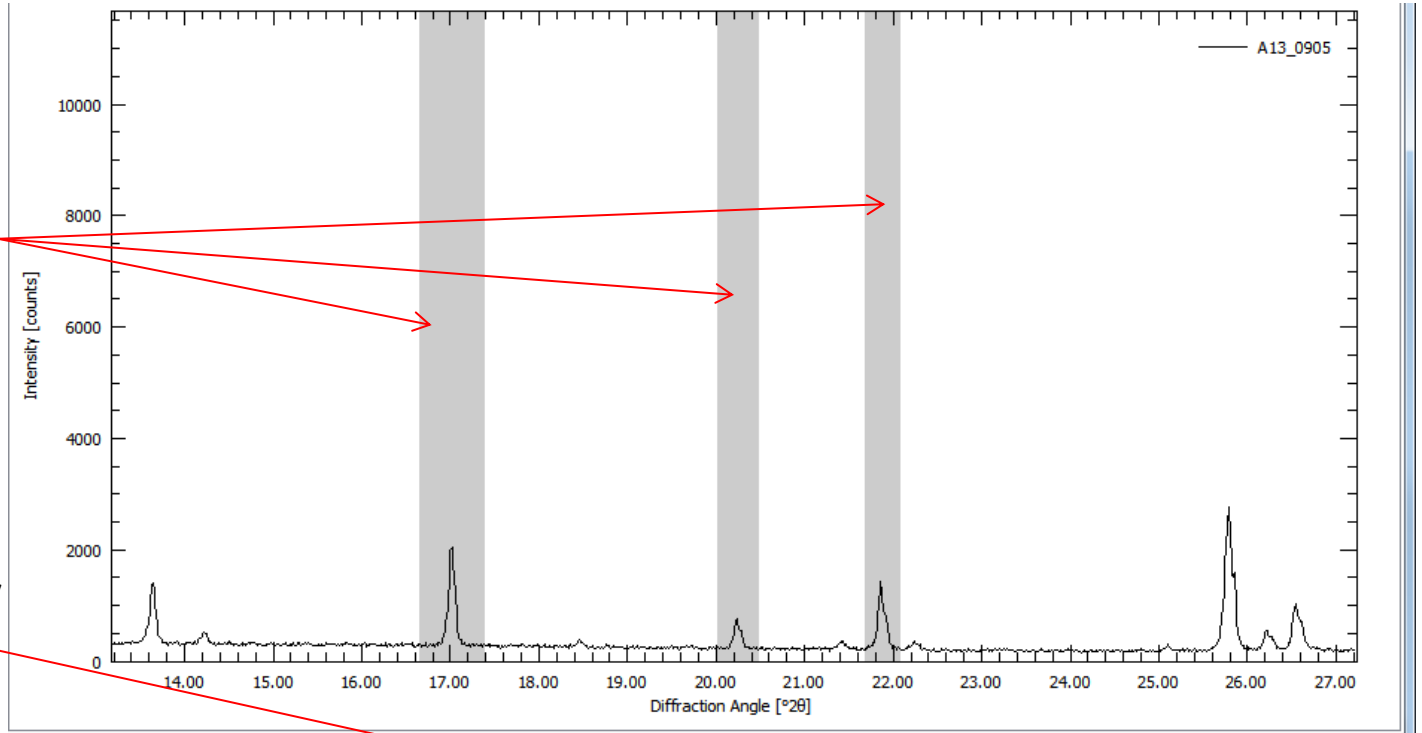



Tools → Scan Math...

# New Tool: Integrate peak intensities

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

2. Integrated intensity
will be calculated



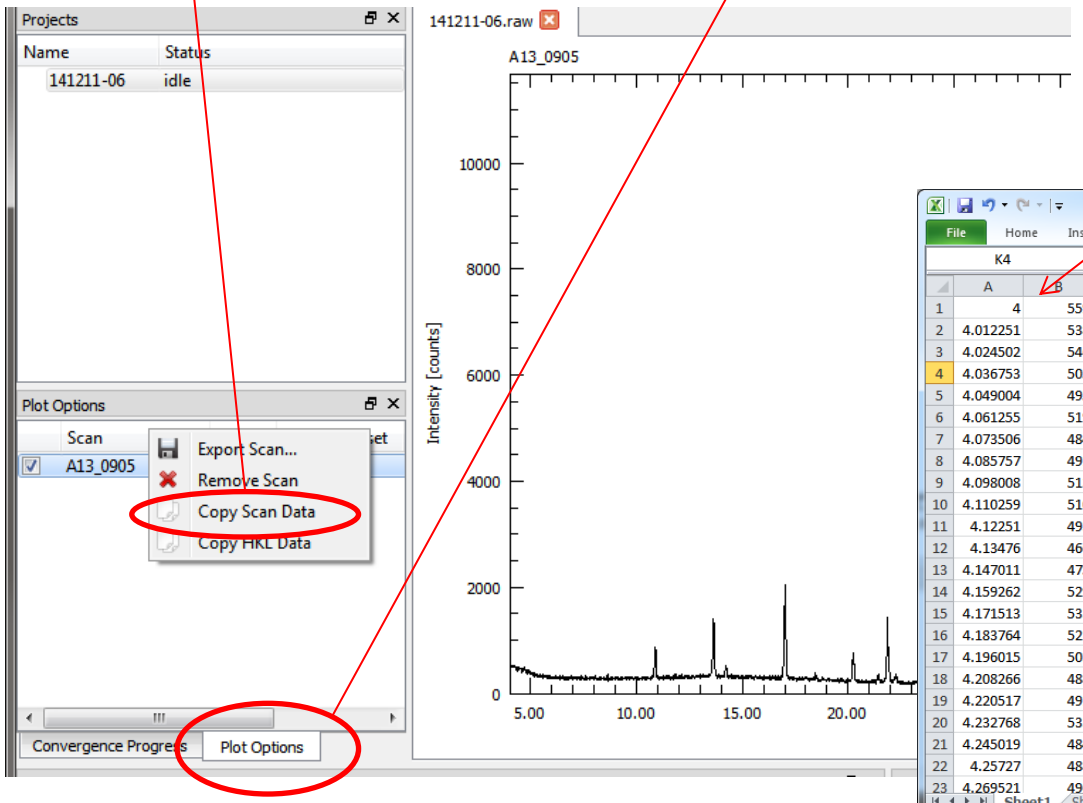

Peak Integrals

| | Range Name | Range Start [°2θ] | Range End [°2θ] | A13_0905 |
|---|---|---|---|---|
| 1 | Range 0 | 16.6629 | 17.3998 | 149.21 |
| 2 | Range 1 | 20.0118 | 20.4996 | 40.96 |
| 3 | Range 2 | 21.6772 | 22.0977 | 120.64 |

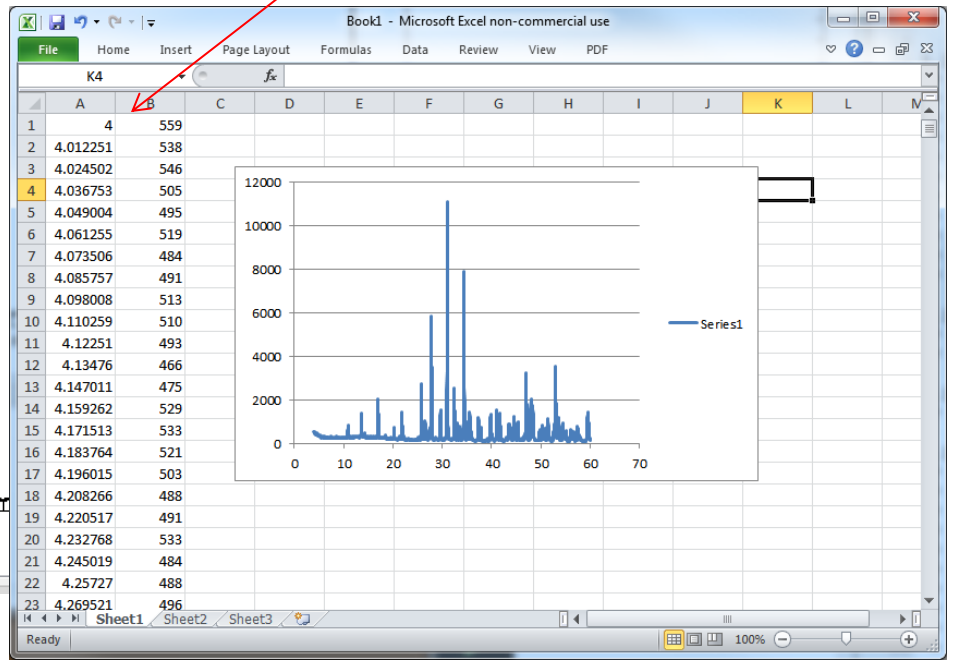
Window → Peak Integrals

# Copy scan data to clipboard

## 1. Right mouse button in Plot Options list

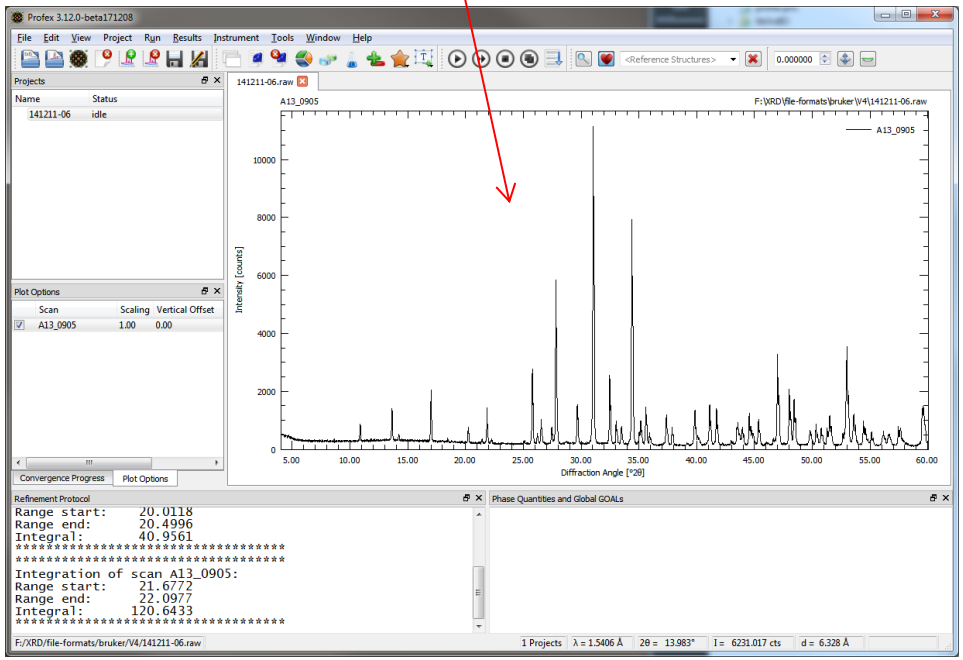



## 2. Paste data to other application

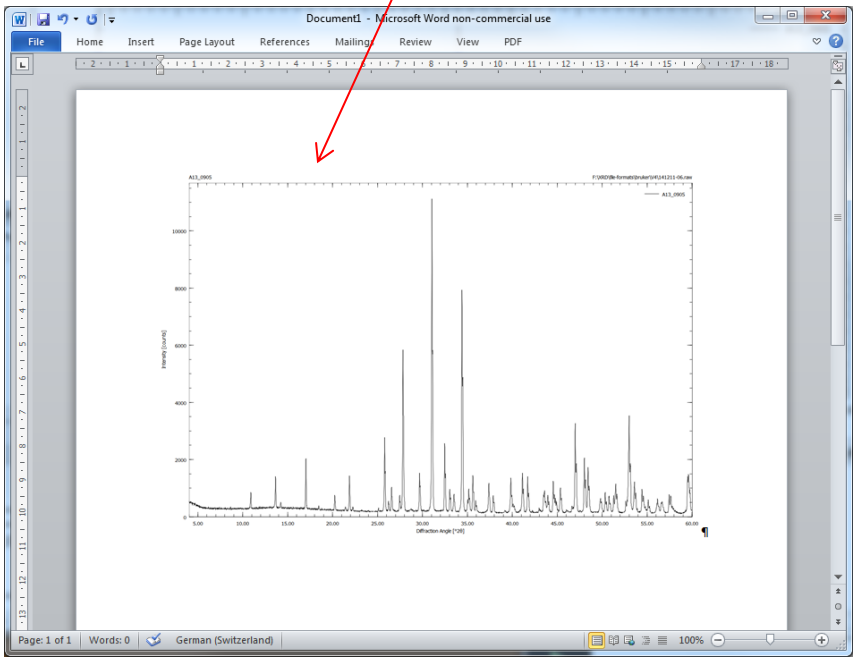


# Copy scan pixel image to clipboard

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




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



# New syntax for quantification GOALs (optional)

01-tutorial.dia | 01-tutorial.sav | 01-tutorial.lst

```
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
```

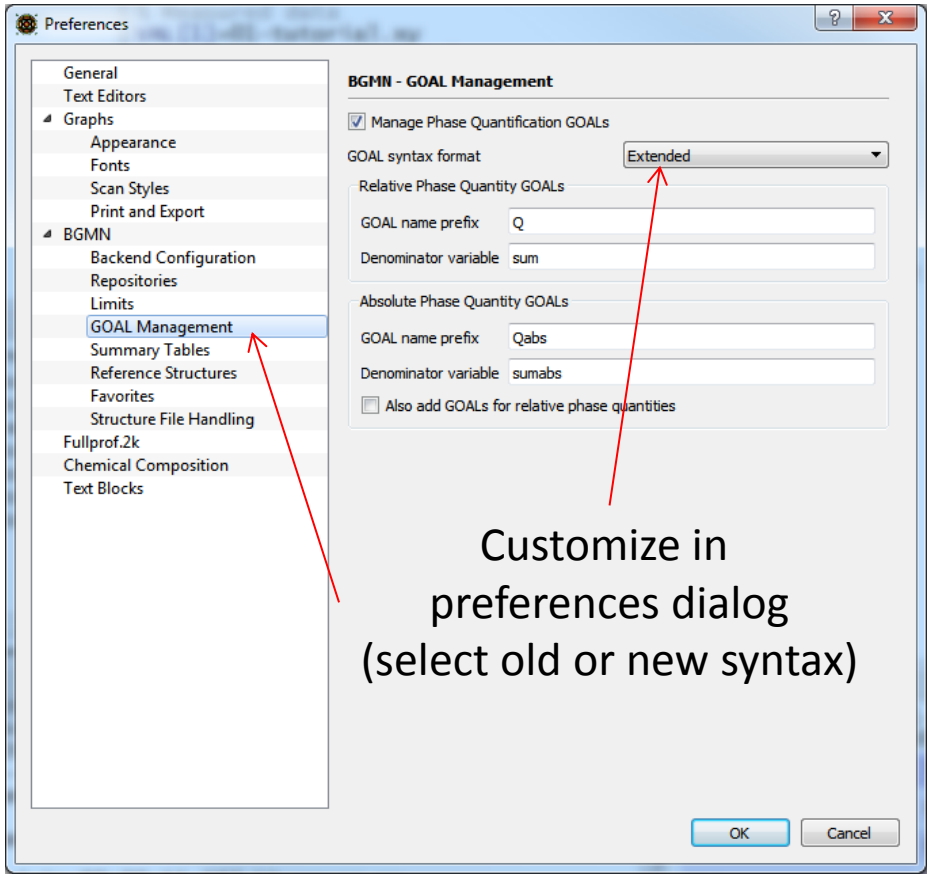
New syntax

Phase Quantities and Global GOALs

F:\XRD\tutorial\01-tutorial.lst
$R_{wp}$=8.53%, $R_{exp}$=7.16%, $X^2$=1.4193 GOF

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

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




Customize in preferences dialog (select old or new syntax)

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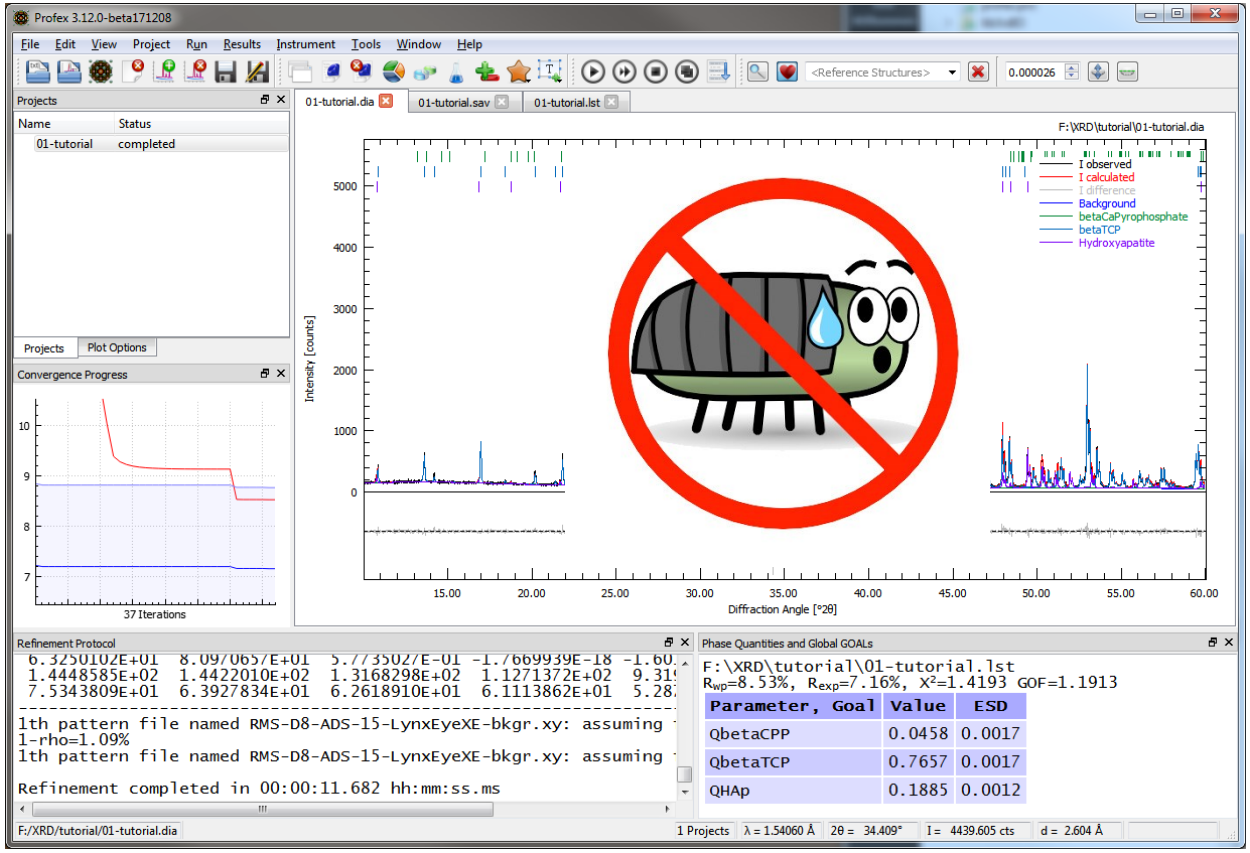
+ many bugfixes




Bug image: http://www.thecomputeradvisor.net