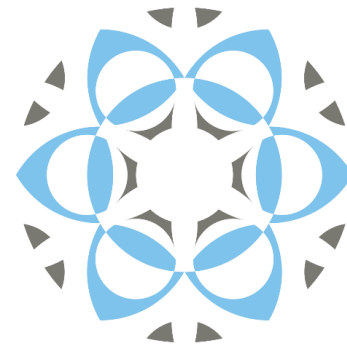


BGMN/Profex User Meeting 2019

New Features in Profex 4 Part 1

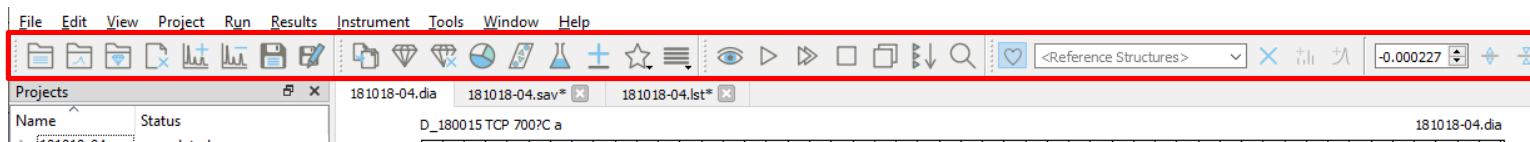
Nicola Döbelin
RMS Foundation, Bettlach, Switzerland

- GUI changes
 - Search / Match
 - Peak detection
 - Interaction with QualX / Match!
-
- Electron-density maps
 - Drawing crystal structures with Vesta / Mercury
 - Customizing report layouts

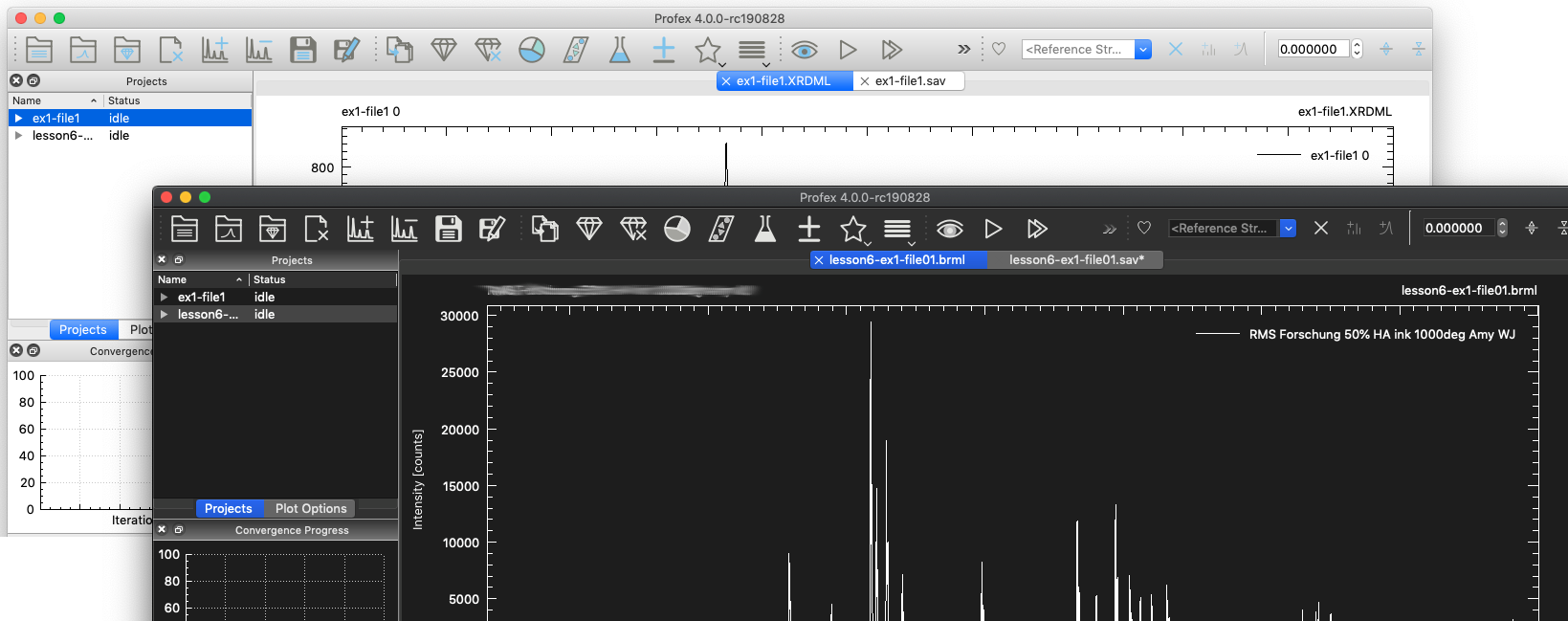


GUI Changes

New icon set:



Support for dark mode on OS X:



Summary tables:

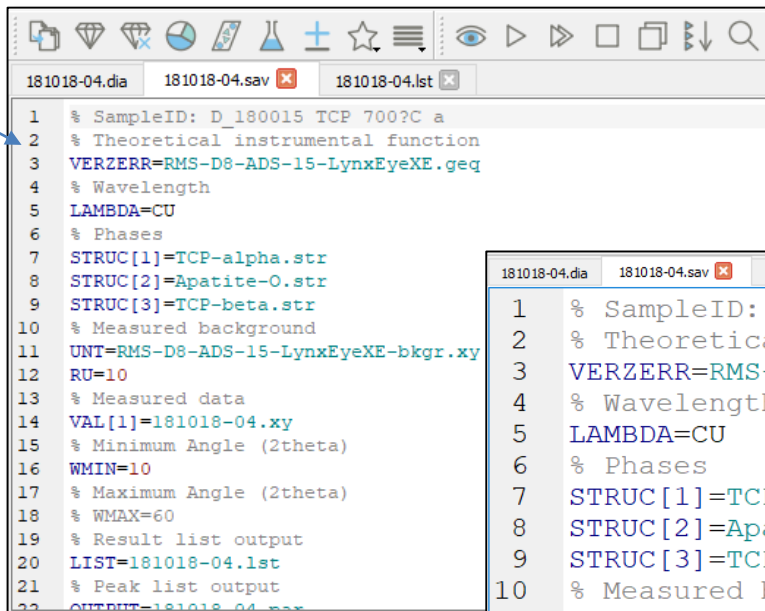
Parameter, Goal	Value	ESD
QHAp	0.09555	0.0013
Qwhitlockite	0.0445	0.0013

Statistics, Global GOALS, and Local GOALS summarized in a tree structure

Parameter	Value	ESD
Statistics		
Rwp	8.03	
Rexp	7.31	
χ^2	1.21	
GoF	1.10	
Global GOALS		
QalphaTCP	0.6299	0.0029
QOxyapatite	0.0605	0.0016
QbetaTCP	0.3095	0.0030
Local GOALS		
alphaTCP		
A	1.28759	0.00009
B	2.7304	0.0001
C	1.52211	0.00007
BETA	126.231	0.004
GrainSize(1,1,1)	98.8	2.6
Oxyapatite		
A	0.94265	0.00009
C	0.68868	0.00009
GrainSize(1,1,1)	79.2	3.2
betaTCP		
A	1.04064	0.00005
C	3.7314	0.0002
GrainSize(1,1,1)	172.0	14.0

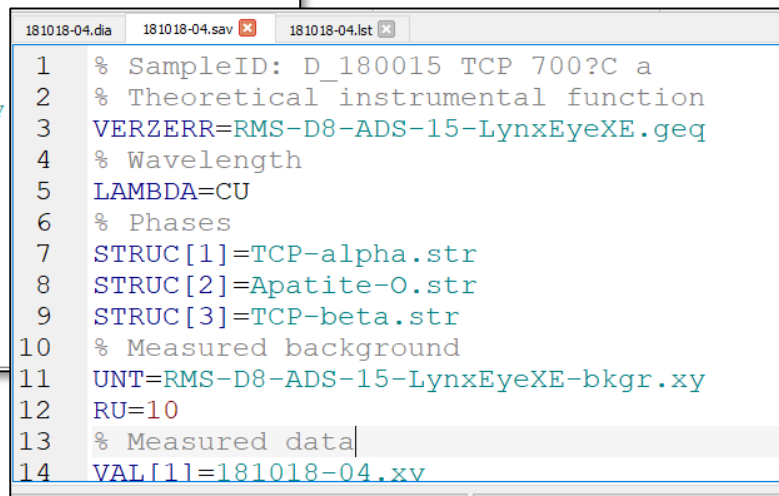
Text editors:

Line numbers



```
1  % SampleID: D_180015 TCP 700?C a
2  % Theoretical instrumental function
3  VERZERR=RMS-D8-ADS-15-LynxEyeXE.geq
4  % Wavelength
5  LAMBDA=CU
6  % Phases
7  STRUC[1]=TCP-alpha.str
8  STRUC[2]=Apatite-O.str
9  STRUC[3]=TCP-beta.str
10 % Measured background
11 UNT=RMS-D8-ADS-15-LynxEyeXE-bkgr.xy
12 RU=10
13 % Measured data
14 VAL[1]=181018-04.xy
15 % Minimum Angle (2theta)
16 WMIN=10
17 % Maximum Angle (2theta)
18 % WMAX=60
19 % Result list output
20 LIST=181018-04.lst
21 % Peak list output
22 OUTDHT=181018-04.max
```

Ctrl + Scroll wheel
changes text size




```
1  % SampleID: D_180015 TCP 700?C a
2  % Theoretical instrumental function
3  VERZERR=RMS-D8-ADS-15-LynxEyeXE.geq
4  % Wavelength
5  LAMBDA=CU
6  % Phases
7  STRUC[1]=TCP-alpha.str
8  STRUC[2]=Apatite-O.str
9  STRUC[3]=TCP-beta.str
10 % Measured background
11 UNT=RMS-D8-ADS-15-LynxEyeXE-bkgr.xy
12 RU=10
13 % Measured data
14 VAL[1]=181018-04.xy
```

Change permanently:

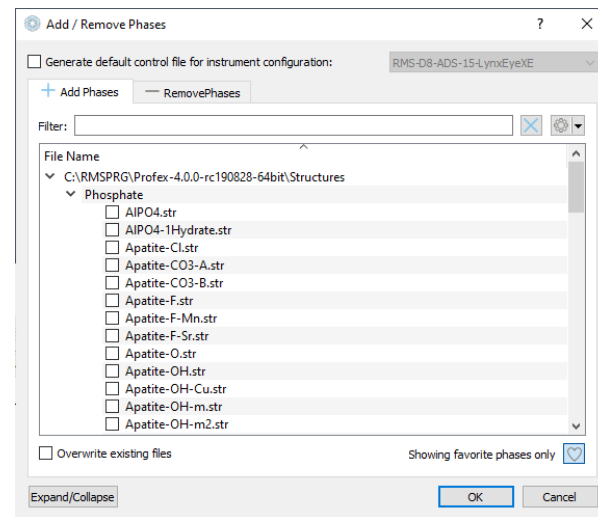
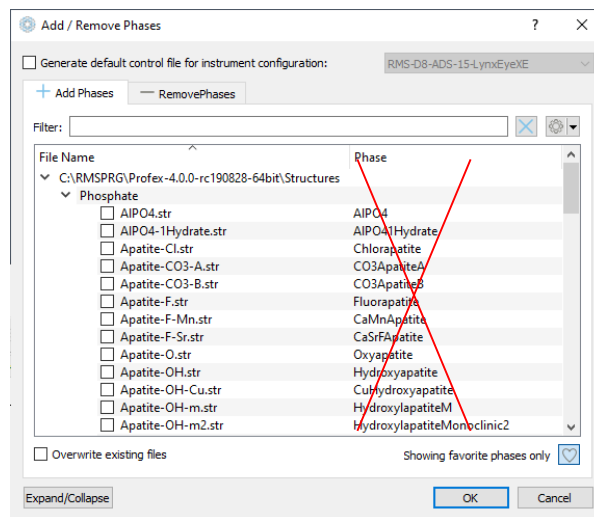
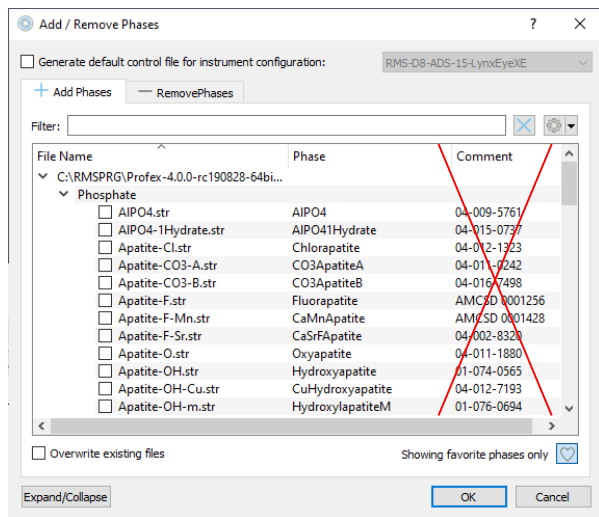
«Edit → Preferences → Text editors»

Spell checker underlines common mistakes:



```
1 PHASE=betaTCP // 04-008-8714
2 MineralName=Whitlockite
3 Formula=Ca3_(PO4)2
4 SpacegroupNo=161 HermannMauguin=R3c
5
6 PARAM=A_1.0439_1.0335^1.0543
7 |
8 PARAM=C=3.7375_3.7380^3.7749
9
10 RP=4 k1=0 PARAM=k2=0_0^0.0001 PARAM=B1=0_0^0.01 GEWICHT=SPHAR6
11 GOAL=GrainSize(1,1,1)
12 GOAL:betaTCP=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1)
13 E=CA Wyckoff=b x=-0.2766 y=-0.1421 z=0.1658 TDS=0.00686924
14 E=CA Wyckoff=b x=-0.3836 y=-0.1775 z=-0.0336 TDS=0.00673765
15 E=CA Wyckoff=b x=-0.2721 y=-0.1482 z=0.0606 TDS=0.01873909
16 E=CA(0.5000) Wyckoff=a x=0.0000 y=0.0000 z=-0.0850 TDS=0.01105396
17 E=CA(0.5000) Wyckoff=b x=0.0000 y=0.0000 z=0.0658 TDS=0.01150120
```

Show / hide certain table columns
(for less information clutter)



Right-click on the table header

New Modules: Search/Match and Peak Detection

Previous versions:

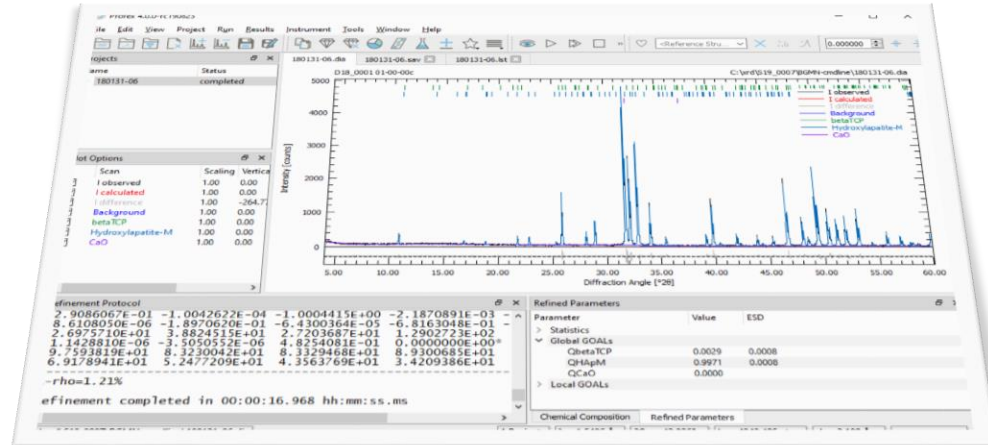
Method	Strengths	Limitations
Double-clicking strongest peak	<ul style="list-style-type: none">• Very fast	<ul style="list-style-type: none">• Fails in case of texture• Internal STR repository only
Scrolling through reference structures	<ul style="list-style-type: none">• Largely unaffected by texture	<ul style="list-style-type: none">• Manual search (tedious)• Internal STR repository only

Profex 4:

Method	Strengths	Limitations
Full-profile search-match (derived from [1])	<ul style="list-style-type: none">• Good hit rate	<ul style="list-style-type: none">• Slow• Internal STR repository only
Peak detection, export to 3 rd party software	<ul style="list-style-type: none">• Searches COD and PDF databases	<ul style="list-style-type: none">• Requires 3rd party software

Full-Profile Search-Match

- Refines each structure file separately
- Uses a restricted refinement strategy (no texture, no anisotropic parameters, limited number of iterations)
- Scores the structure files by the refinement statistics (Figure of Merit, FoM) (see Profex User Manual Part 2)
- Requires a correct instrument configuration



Full-Profile Search-Match

1

2

3

Profex 4.0.0-rc190826

File Edit View Project Run Results Instrument Window Help

Projects

Name	Status
JC_KS_MC	idle

Plot Options

Scan	Scaling	Vertical Offset
<input checked="" type="checkbox"/> JC_KS_MC 0	1.00	0.00

Search/Match Phases

Database Controls Results

Favorites 73

Directories 752

Repository	Number of phases
<input type="checkbox"/> C:\RMS\PRG\Profex-4.0.0-rc19...	1
<input type="checkbox"/> SIC	26
<input type="checkbox"/> Phosphate	73
<input type="checkbox"/> Organic	12
<input type="checkbox"/> Minerals	76
<input type="checkbox"/> MetalsAlloysOxides	24
<input type="checkbox"/> Ceramics	99
<input type="checkbox"/> Cement	12
<input type="checkbox"/> BGMN	412
<input type="checkbox"/> Alumina-Titania-Zirconia...	17

Intensity [counts]

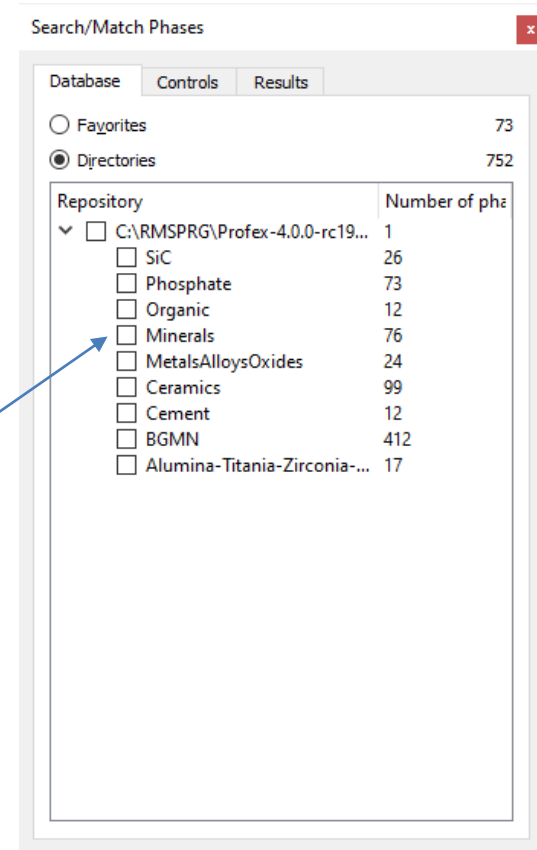
Diffraction Angle [°2Theta]

1 Project $\lambda = 1.5406 \text{ \AA}$ $2\theta = 0.000^\circ$ $I = 0.000 \text{ cts}$ $d = 0.000 \text{ \AA}$

Page «Database»:

- Select the subset of the Profex structure file Repository to be searched.
- Searching among all 752 structures will take a long time...

For our example: Check «Minerals»



Full-Profile Search-Match

Page «Controls»:

- Select the instrument configuration used to measure the dataset.
- Select the wavelength distribution.
- Specify the number of iterations and angular range to be used for phase matching.

For our example:

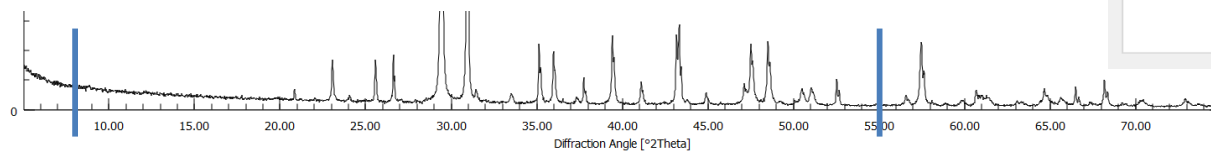
Instrument = xpert-xcel-fds-0250

Radiation = CU

Number of iterations = 15

Minimum angle = 8.0

Maximum angle = 55.0



Search/Match Phases

Database

Controls

Results

Instrument configuration xpert-xcel-fds-0250

Characteristic Radiation CU

Synchrotron Radiation 0.0500000 nm

Number of Iterations 15

Minimum Angle 8.00

Maximum Angle 55.00

Allow anisotropic parameters

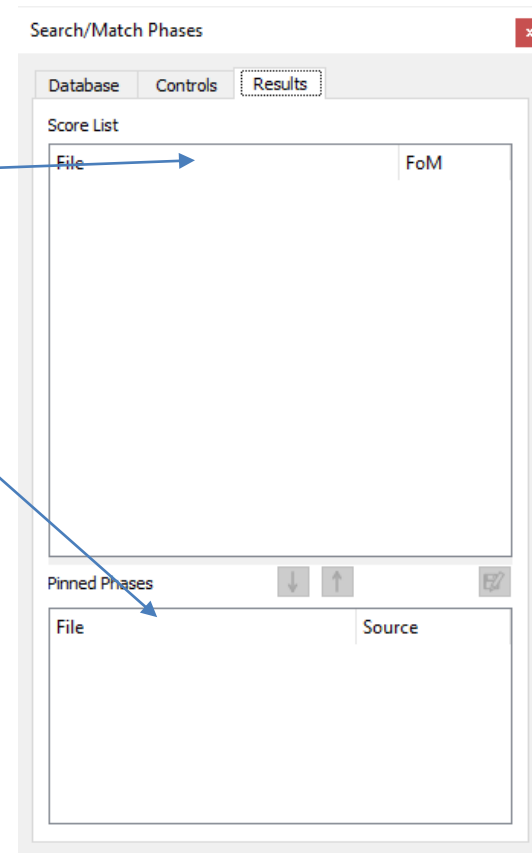
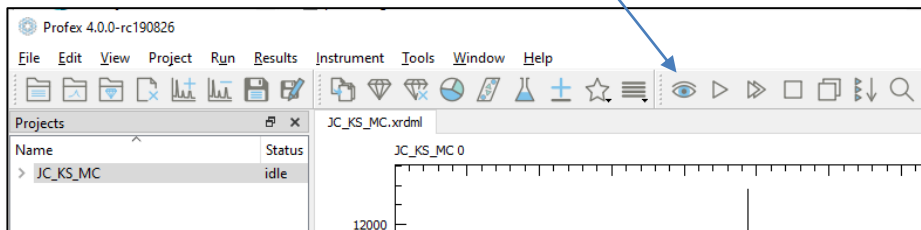
Refine sample height displacement

Full-Profile Search-Match

Page «Results»:

- No results yet
- Columns «Phase» and «Fraction» can be hidden (right mouse button)

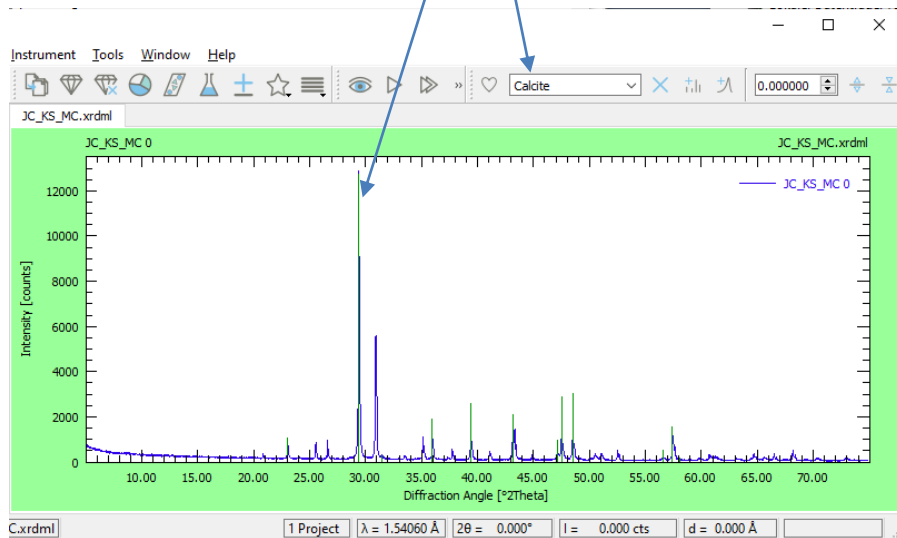
Start Search/Matching:



Full-Profile Search-Match

Page «Results»:

- Best matches appear on top of the list
- Absolute FoM has no meaning, varies strongly from dataset to dataset
- Click on phase to show hkl lines



Search/Match Phases

Database Controls Results

Score List

File	FoM
Calcite.str	0.096061
Dolomite.str	0.045640
Corundum.str	0.044943
Arcanite.str	0.041963
Troemelite.str	0.035226
Periclastr	0.034704
Fluorite.str	0.027076
Turmaline-Schorl.str	0.026858
Gyrolite.str	0.026599
Muscovite2M1.str	0.025750
Wollastonite1A.str	0.025408
Graphite-3r.str	0.023557
Shlykovite.str	0.023391
Newberyite.str	0.022614
Kaolinite-1A.str	0.022324

Pinned Phases

File	Source

Full-Profile Search-Match

Page «Results»:

- To accept matches, select the file and pin it

Run Search/Match again to perform a residual search



Search/Match Phases

Database Controls Results

Score List

File	FoM
Corundum.str	0.044943
Arcanite.str	0.041963
Troemelite.str	0.035226
Periclase.str	0.034704
Fluorite.str	0.027076
Turmaline-Schorl.str	0.026858
Gyrolite.str	0.026599
Muscovite2M1.str	0.025750
Wollastonite1A.str	0.025408
Graphite-3r.str	0.023557
Shlykovite.str	0.023391
Newberyite.str	0.022614
Kaolinite1A.str	0.022324
Zincite.str	0.021820
Magnetite.str	0.021716

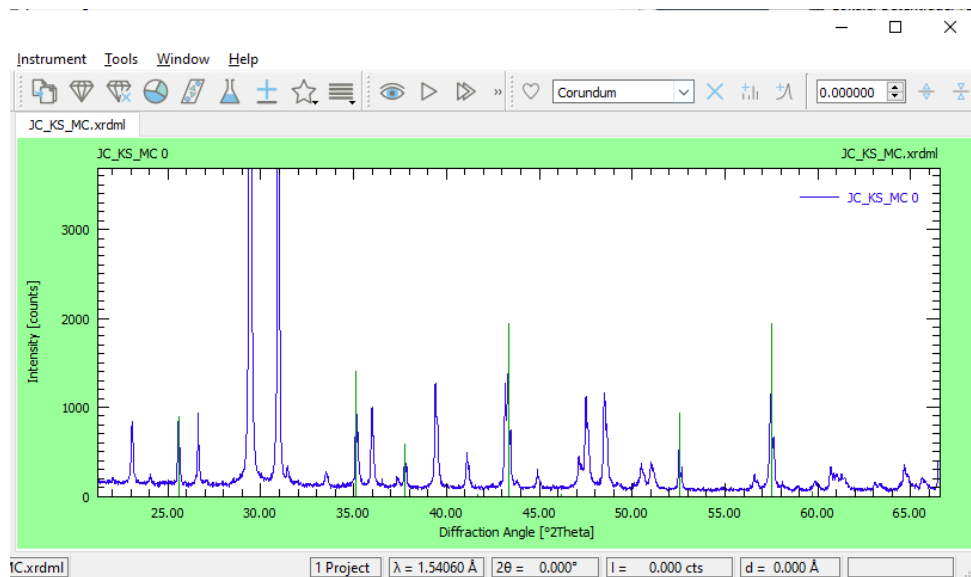
Pinned Phases

File	Source
Calcite.str	matched
Dolomite.str	matched

Full-Profile Search-Match

Page «Results»:

- Residual search results
- Pin Corundum.str
- Run another residual search...



Search/Match Phases

Database Controls Results

Score List

File	FoM
Corundum.str	0.070128
Muscovite2M1.str	0.046731
Arcanite.str	0.045005
Periclase.str	0.043915
Graphite-3r.str	0.043401
Graphite-2h.str	0.040947
Quartz-p3221.str	0.040619
Wollastonite1A.str	0.040591
Magnetite.str	0.040459
Turmaline-Schorl.str	0.040428
Clinochlore1A.str	0.039678
Ganophyllite.str	0.039598
Shlykovite.str	0.039288
Quartz-p3121.str	0.039055
...	...

Pinned Phases

File	Source
Calcite.str	matched
Dolomite.str	matched

Full-Profile Search-Match

Page «Results»:

- Arcanite is a false positive due to proximity of dolomite peaks.
- Final match list:

Search/Match Phases

Database Controls Results

Score List


File	FoM
Arcanite.str	0.054853
Katoite.str	0.051196
Tuite.str	0.051151
Struvite.str	0.051033
Gypsum.str	0.050835
Albite.str	0.050556
Anhydrite.str	0.050556
Ardealite.str	0.050556
Biotite1M.str	0.050556
Cristobalite.str	0.050556
Diamond.str	0.050556
Ettringite.str	0.050556
Glauconite.str	0.050556
Hematite.str	0.050556
Libanite.str	0.050556

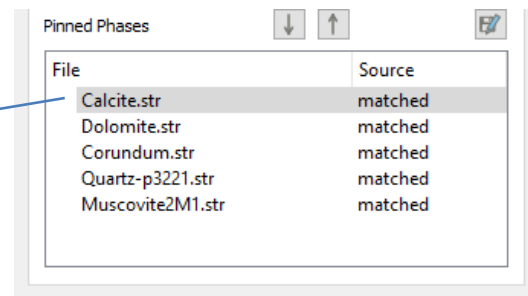
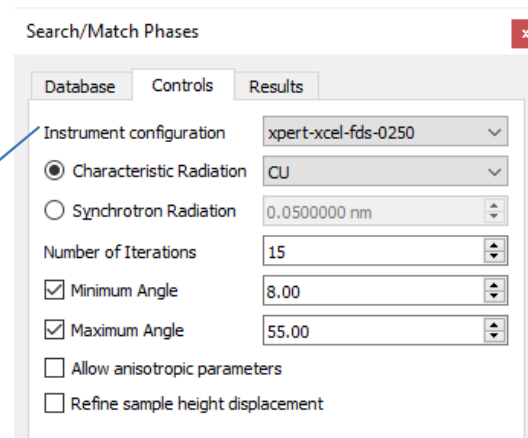
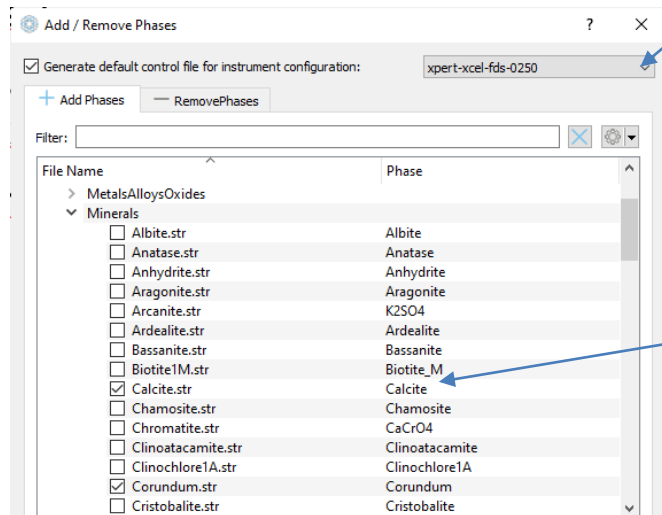
Pinned Phases

File	Source
Calcite.str	matched
Dolomite.str	matched
Corundum.str	matched
Quartz-p3221.str	matched
Muscovite2M1.str	matched

Full-Profile Search-Match

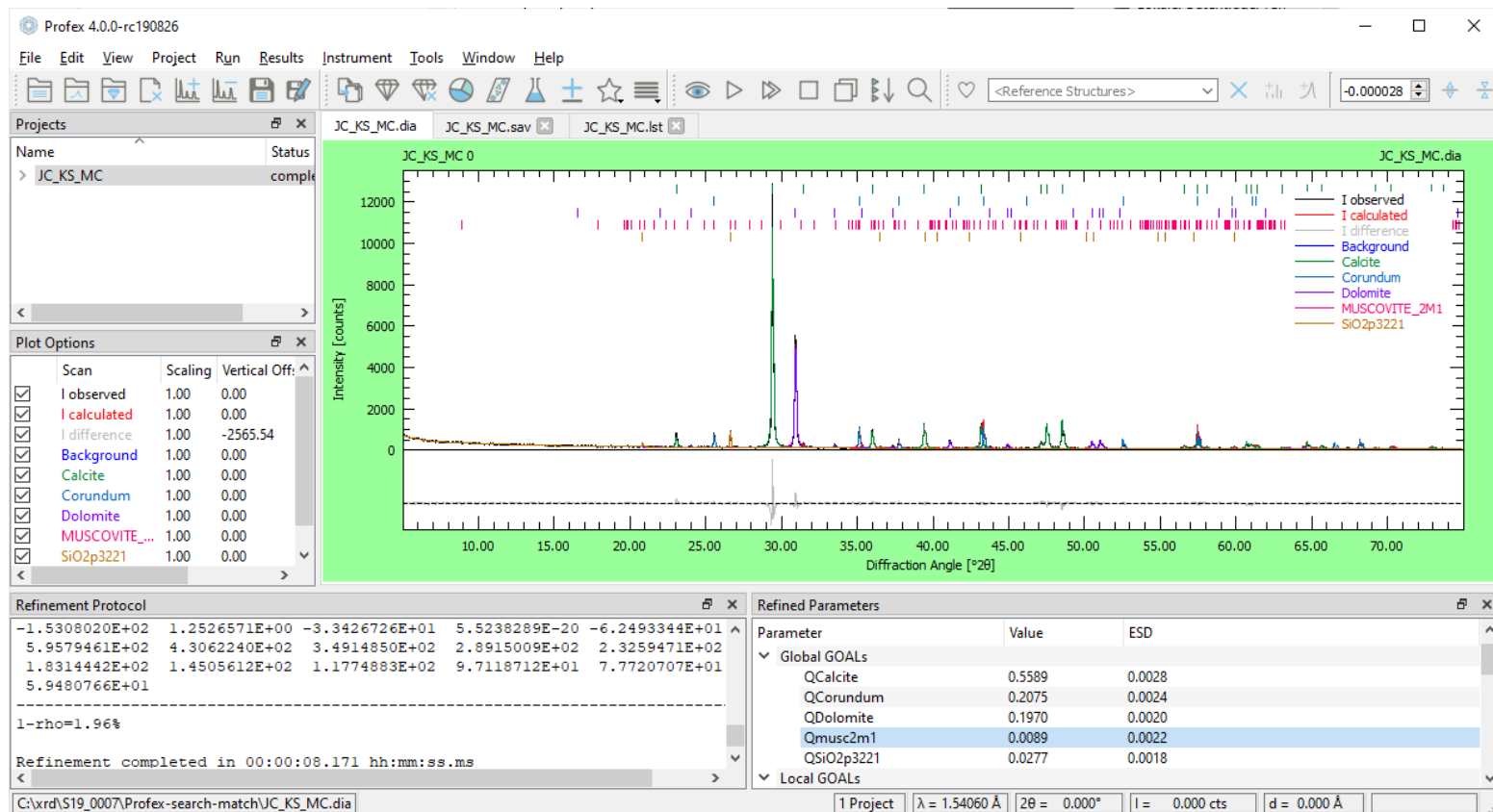
Page «Results»:

- Create a refinement project from the pinned phases: 
- Instrument settings are applied and pinned phases are pre-selected



Full-Profile Search-Match

Refinement can be started immediately...

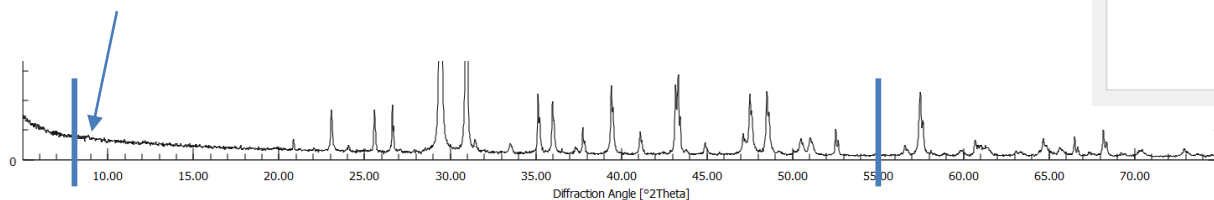


Full-Profile Search-Match

Speed up the process:

- Reduce number of iterations (typically 10 – 15)
- Increase minimum angle to just below the first observed peak
- Reduce maximum angle

Do not clip low-angle peaks!



Search/Match Phases

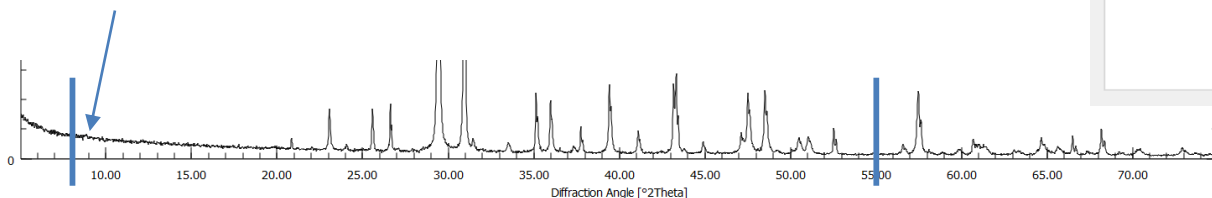
Database	Controls	Results
Instrument configuration	xpert-xcel-fds-0250	
<input checked="" type="radio"/> Characteristic Radiation	CU	
<input type="radio"/> Synchrotron Radiation	0.0500000 nm	
Number of Iterations	15	
<input checked="" type="checkbox"/> Minimum Angle	8.00	
<input checked="" type="checkbox"/> Maximum Angle	55.00	
<input type="checkbox"/> Allow anisotropic parameters		
<input type="checkbox"/> Refine sample height displacement		

Full-Profile Search-Match

Improve hit rate:

- Strongly textured samples may benefit from refining anisotropic parameters.
- Strongly displaced samples may require refinement of height displacement.

Both options often increase the number of false positive matches.
Only activate for residual search.



Search/Match Phases

Database	Controls	Results
Instrument configuration	xpert-xcel-fds-0250	
<input checked="" type="radio"/> Characteristic Radiation	CU	
<input type="radio"/> Synchrotron Radiation	0.0500000 nm	
Number of Iterations	15	
<input checked="" type="checkbox"/> Minimum Angle	8.00	
<input checked="" type="checkbox"/> Maximum Angle	55.00	
<input type="checkbox"/> Allow anisotropic parameters		
<input type="checkbox"/> Refine sample height displacement		

Full-Profile Search-Match

Search/Match Phases

Database Controls Results

Score List

File	FoM
Arcanite.str	0.054853
Katoite.str	0.051196
Tuite.str	0.051151
Struvite.str	0.051033
Gypsum.str	0.050835
Albite.str	0.050556
Anhydrite.str	0.050556
Ardealite.str	0.050556
Biotite1M.str	0.050556
Cristobalite.str	0.050556
Diamond.str	0.050556
Ettringite.str	0.050556
Glauconite.str	0.050556
Hematite.str	0.050556
Ulexite.str	0.050556

Pinned Phases

File	Source
Calcite.str	matched
Dolomite.str	matched
Corundum.str	matched
Quartz-p3221.str	matched
Muscovite2M1.str	matched

Final residual search:

Anisotr. not allowed

Anisotr. allowed

Search/Match Phases

Database Controls Results

Instrument configuration: xpert-xcel-fds-0250

Characteristic Radiation: CU

Synchrotron Radiation: 0.0500000 nm

Number of Iterations: 15

Minimum Angle: 8.00

Maximum Angle: 55.00

Allow anisotropic parameters

Refine sample height displacement

Search/Match Phases

Database Controls Results

Score List

File	FoM
Albite.str	0.105820
Anhydrite.str	0.105820
Cristobalite.str	0.105820
Ettringite.str	0.105820
Leucite.str	0.105820
Quartz-p3121-HP.str	0.105820
Spinel.str	0.105820
Lime.str	0.105721
Merrillite.str	0.105708
Periclase.str	0.105708
Rutile.str	0.105708
Wollastonite-Pseudo.str	0.105708
Diamond.str	0.104725
Gypsum.str	0.104395
Katoite.str	0.103330

Pinned Phases

File	Source
Calcite.str	matched
Dolomite.str	matched
Corundum.str	matched
Muscovite2M1.str	matched
Quartz-p3221.str	matched

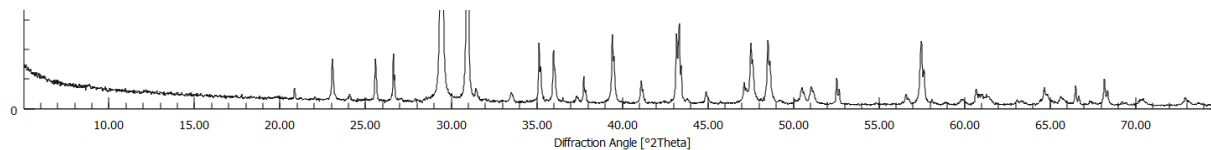
Full-Profile Search-Match

Summary:

- Full-profile search-match with good hit rate
- Excellent residual search hit rate
- Easily create refinement projects from matched phases



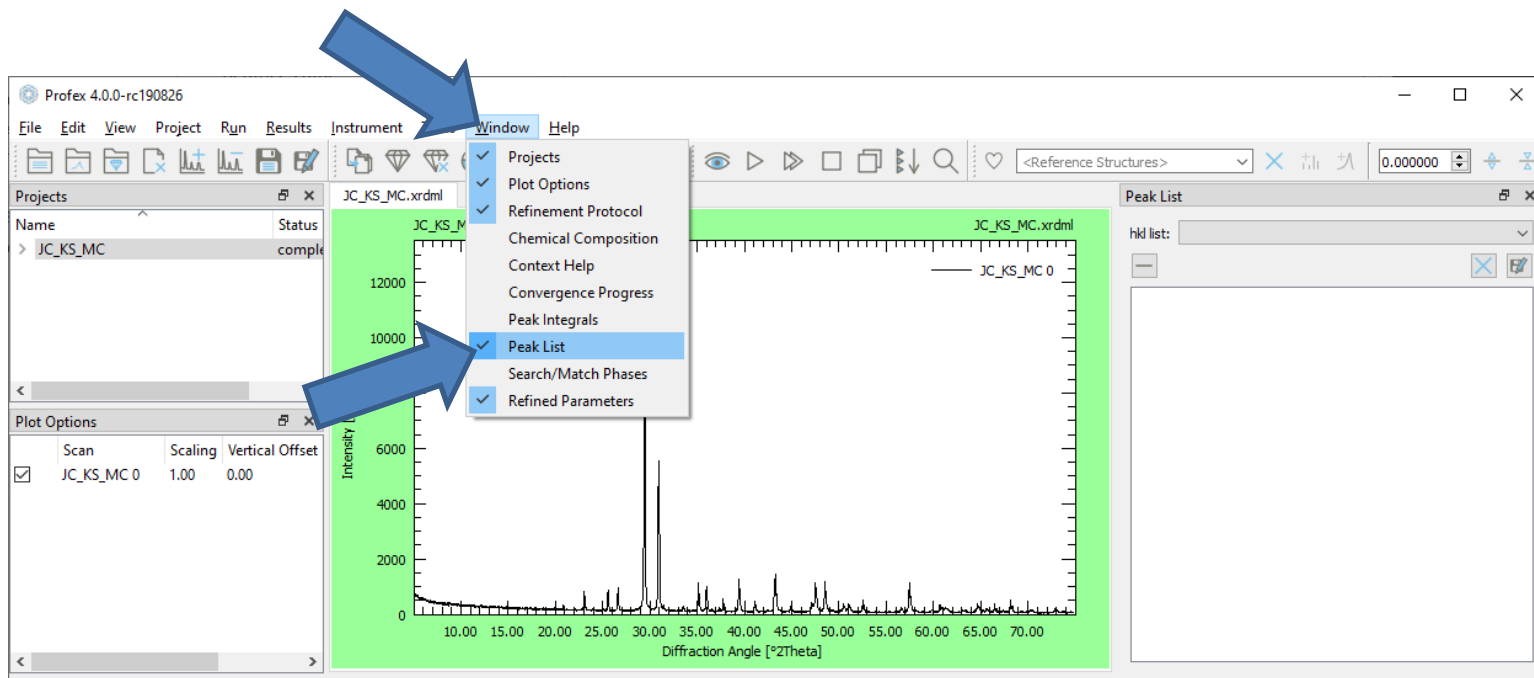
- Slow
- Only searches internal structure repository



Search/Match Phases		
Database	Controls	Results
Score List		
File		FoM
Albite.str		0.105820
Anhydrite.str		0.105820
Crystobalite.str		0.105820
Ettringite.str		0.105820
Leucite.str		0.105820
Quartz-p321-HP.str		0.105820
Spinel.str		0.105820
Lime.str		0.105721
Merrillite.str		0.105708
Periclase.str		0.105708
Rutile.str		0.105708
Wollastonite-Pseudo.str		0.105708
Diamond.str		0.104725
Gypsum.str		0.104395
Calcite.str		0.104395
Pinned Phases		
File	Source	
Calcite.str	matched	
Dolomite.str	matched	
Corundum.str	matched	
Muscovite2M1.str	matched	
Quartz-p3221.str	matched	

Peak Detection

Peak detection with EFLECH (part of BGMN)
Export peak list to 3rd party Search/Match software



Peak Detection

1

2

3

4

Profex 4.0.0-1

File Edit View Project Run Results Instrument Tools Window Help

Run Search-Match
Run Refinement F9
Run Batch Refinement F10
Abort Current Refinement Shift+F9
Abort All Refinements Shift+F10
Run Peak Detection
Follow Active Refinement

Projects

Name

JC_KS_MC

Plot Options

Scan	Scaling	Vertical Offset
JC_KS_MC 0	1.00	0.00

Intensity [counts]

8000
6000
4000
2000
0

10.00 15.00 20.00 25.00 30.00 35.00

Diffraction

JC_KS_MC.xrdml

JC_KS_MC 0

Peak List

hkl list:

Select Instrument Configuration

Instrument Configuration File xpert-xcel-fds-0250

Wavelength

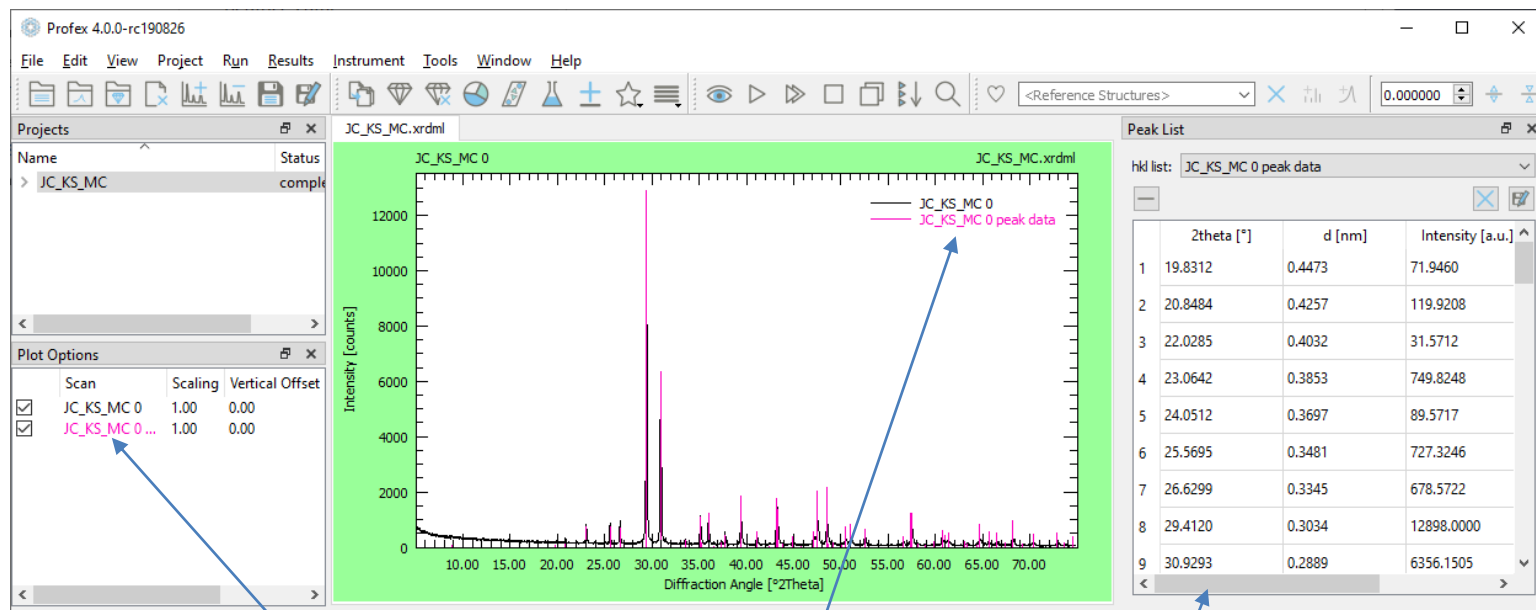
Characteristic CU

Synchrotron 0.070000 nm

OK Cancel

For our example:
Instrument: xpert-xcel-fds-0250
Wavelength: Characteristic CU

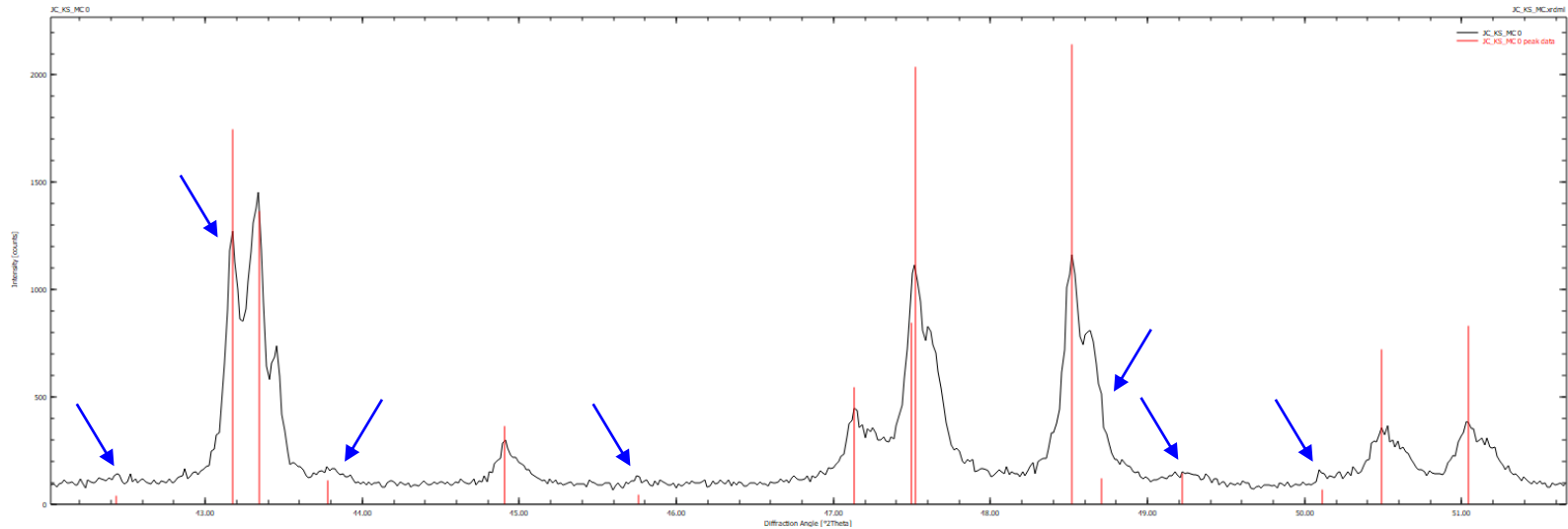
Peak Detection



List of detected peaks is appended as a new hkl scan

Peak Detection

- Correct identification of $K\alpha_2$ and $K\beta$ peaks
- Outstanding deconvolution of overlapping peaks
- Very sensitive to low-intensity peaks



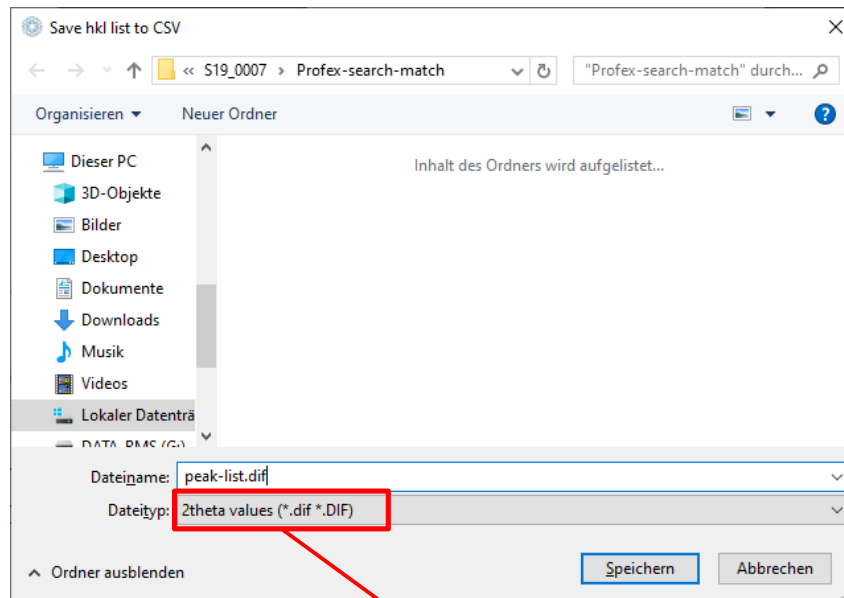
Peak Detection

Peak List

hkl list: JC_KS_MC 0 peak data

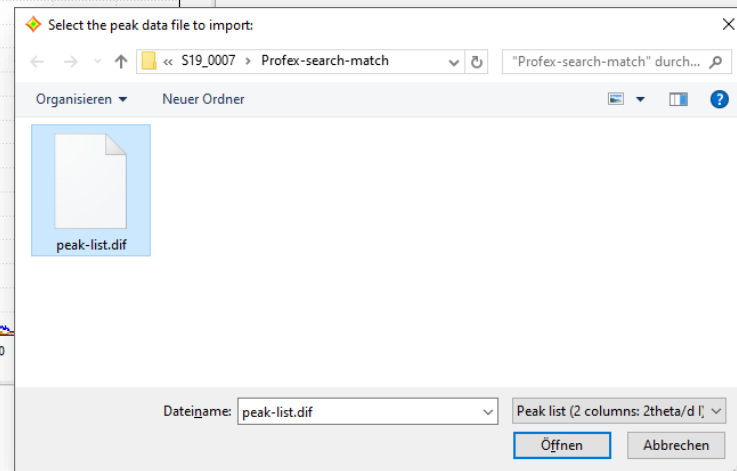
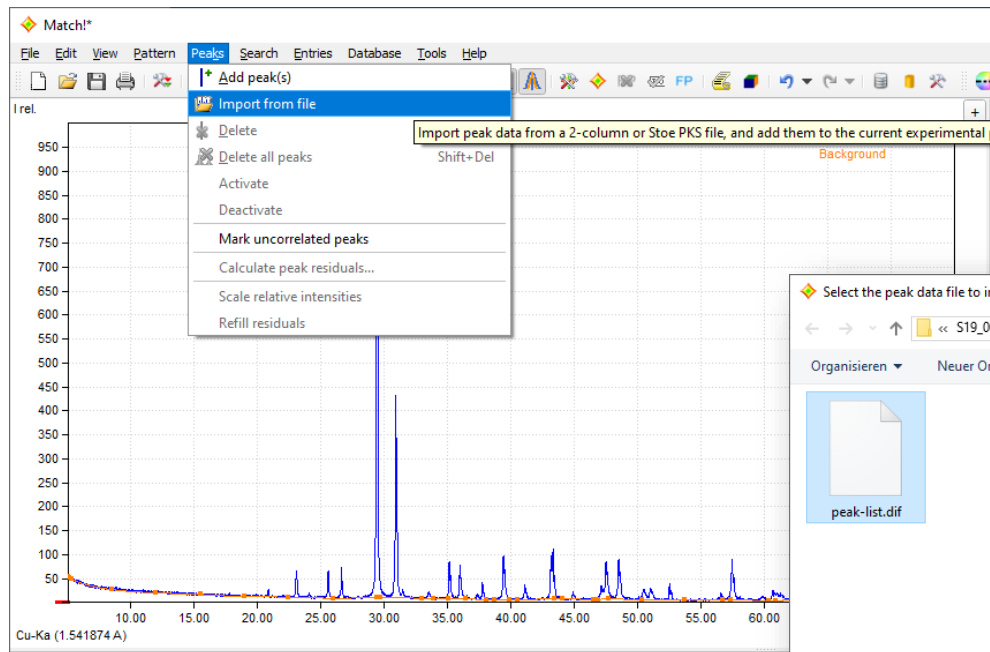
	2theta [°]	d [nm]	Intensity [a.u.]
1	19.8312	0.4473	71.9460
2	20.8484	0.4257	119.9208
3	22.0285	0.4032	31.5712
4	23.0642	0.3853	749.8248
5	24.0512	0.3697	89.5717
6	25.5695	0.3481	727.3246
7	26.6299	0.3345	678.5722
8	29.4120	0.3034	12898.0000
9	30.9293	0.2889	6356.1505
10	33.5049	0.2672	231.2011
11	35.1395	0.2552	1093.2758
12	35.2735	0.2542	141.1452
13	35.9862	0.2494	1211.9070
14	36.5304	0.2458	35.0244

Save peak list to file



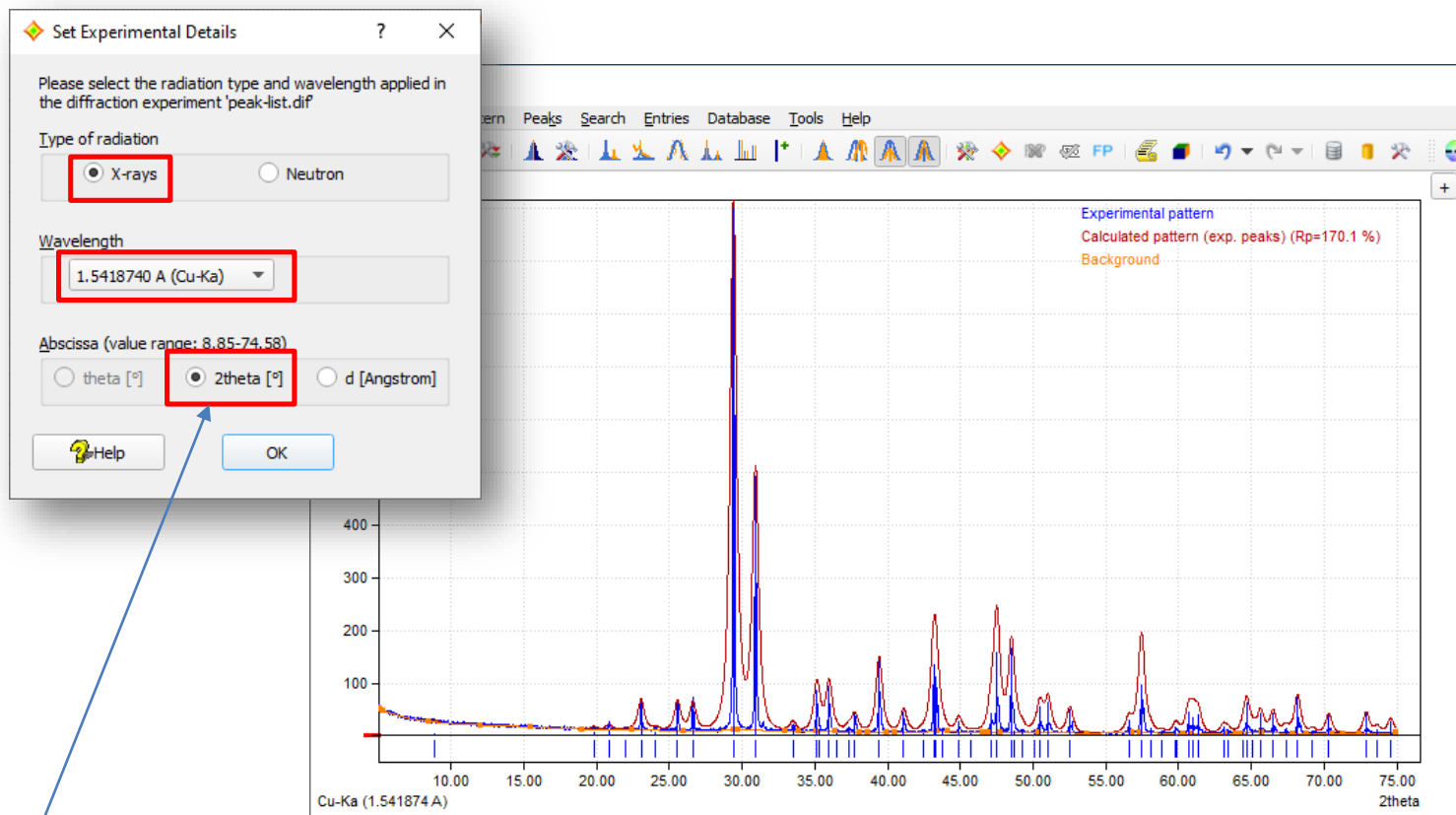
Set format to «2theta values (*.dif)»

Import Peak List in Match!



1. Open scan file
2. Select «Peaks → Import from file»
3. Format «Peak list (2 columns: 2theta/d I)»

Import Peak List in Match!



When exported as «d values (*.dif)» from Profex,
select «d [Angstrom]» here.

Import Peak List in Match!

Match!*

File Edit View Pattern Peaks Search Entries Database Tools Help

Find phases/entries

Experimental pattern
Calculated pattern (exp. peaks) (Rp=62.2 %)
Background
[01-085-0849] Ca (C O3) Calcium Carbonate Calcite, syn (47.9%)
[01-081-8226] Ca Mg (C O3)2 Calcium Magnesium Carbonate Dolomite (31.9%)
[04-004-5100] Al2 O3 Aluminum Oxide Corundum, syn (20.1%)
[01-085-0457] Si O2 Silicon Oxide (Quartz, syn)

Composition* Structure Properties Peaks/Ranges References Su

1a 2a 3b 4b 5b 6b 7b 8b 1b 2b 3a 4a 5a 6a 7a 8a

P1 H He
P2 Li Be B C N O F Ne
P3 Na Mg Al Si P S Cl Ar
P4 K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr
P5 Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe
P6 Cs Ba La Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn
P7 Fr Ra Ac

L Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu
A Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr

Element selection by mouse
 All None Any Optional
 Inorganics only (no C-H-bonds)
 Name:
 Elem. count:
 Formula sum:
 Preset:

Restraints (44433)

Color	Qual.	Entry	Formula	Candidate phase	P(2theta)	P(I/I0)	I scale fct.	I/Ic	FoM
I	04-003-4495	Ti N	Titanium Nitride (Osbornite, syn)	0.6067	0.8306	0.0711	4.08	0.6701	
I	01-076-6599	Mg O	Magnesium Oxide	0.5303	0.9959	0.0514	3.06	0.6674	
I	01-085-0625	Fe0.942 O	Iron Oxide	0.5473	0.9978	0.0468	4.75	0.6656	
I	04-021-1221	Fe0.30 Ni0.32 Al0...	Aluminum Iron Nickel (Steinhardtite)	0.5194	0.9992	0.0525	7.87	0.6618	
*	01-083-0539	Si O2	Silicon Oxide (Quartz, syn)	0.5276	0.8768	0.0549	3.07	0.6611	
I	04-018-2594	Ge0.07 Si0.93 O2	Germanium Silicon Oxide	0.5207	0.8755	0.0551	3.25	0.6598	
I	04-018-2596	Ge0.13 Si0.87 O2	Germanium Silicon Oxide	0.4879	0.8644	0.0586	3.43	0.6576	
I	01-085-0457	Si O2	Silicon Oxide (Quartz, syn)	0.5006	0.8778	0.0562	2.99	0.6575	
B	01-070-2517	Si O2	Silicon Oxide (Quartz, syn)	0.5199	0.8937	0.0494	3.03	0.6569	

Color Entry Formula Matched phase Quant.(%)
 01-085-0849 Ca (C O3) Calcium Carbonate Calcite, syn 47.9
 01-081-8226 Ca Mg (C O3)2 Calcium Magnesium Carbonate... 31.9
 04-004-5100 Al2 O3 Aluminum Oxide Corundum, syn 20.1

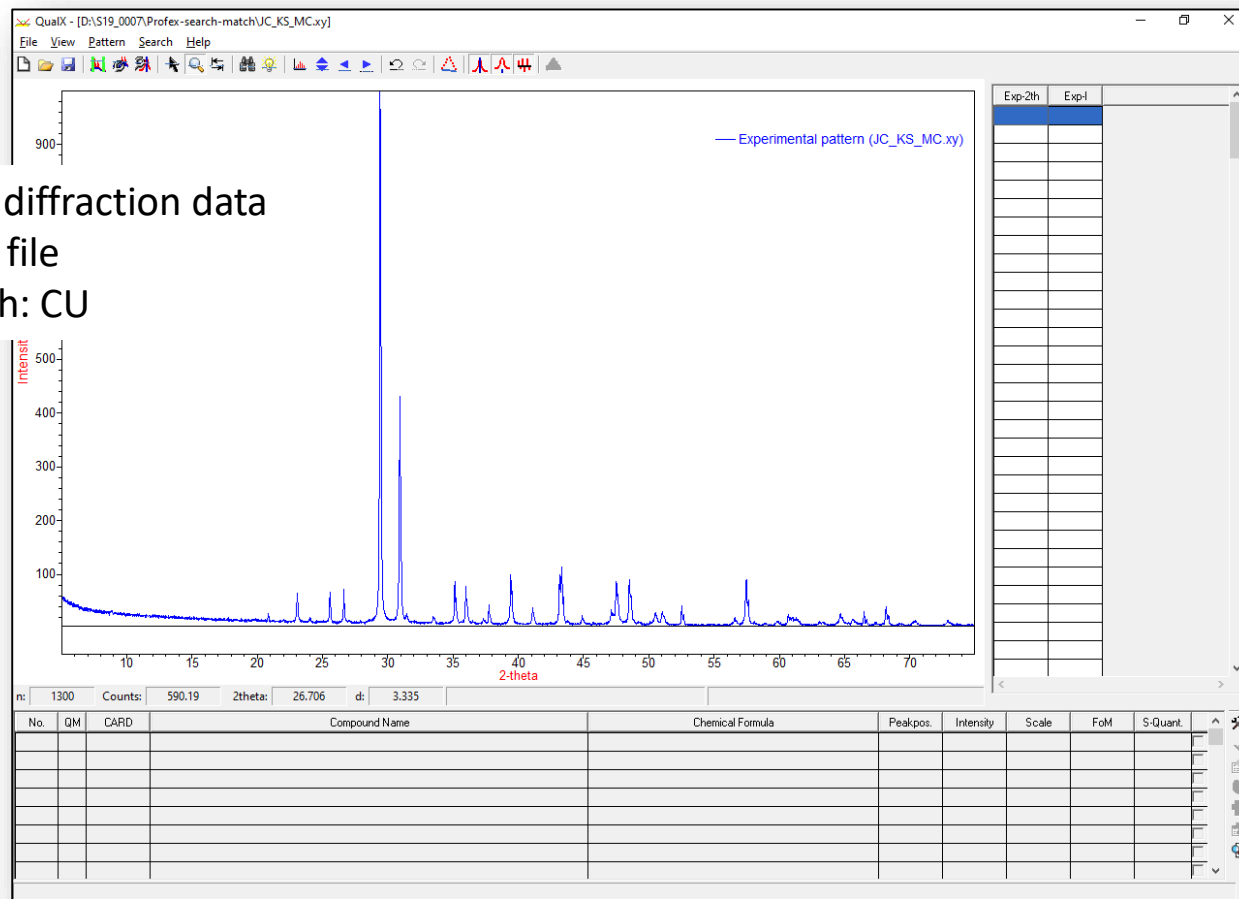
2th: 59.70 d: 1.5490 I rel.: 1000.00 134 entries PDF-4+ 2019 RDB

Robert Mathys Foundation, Site License

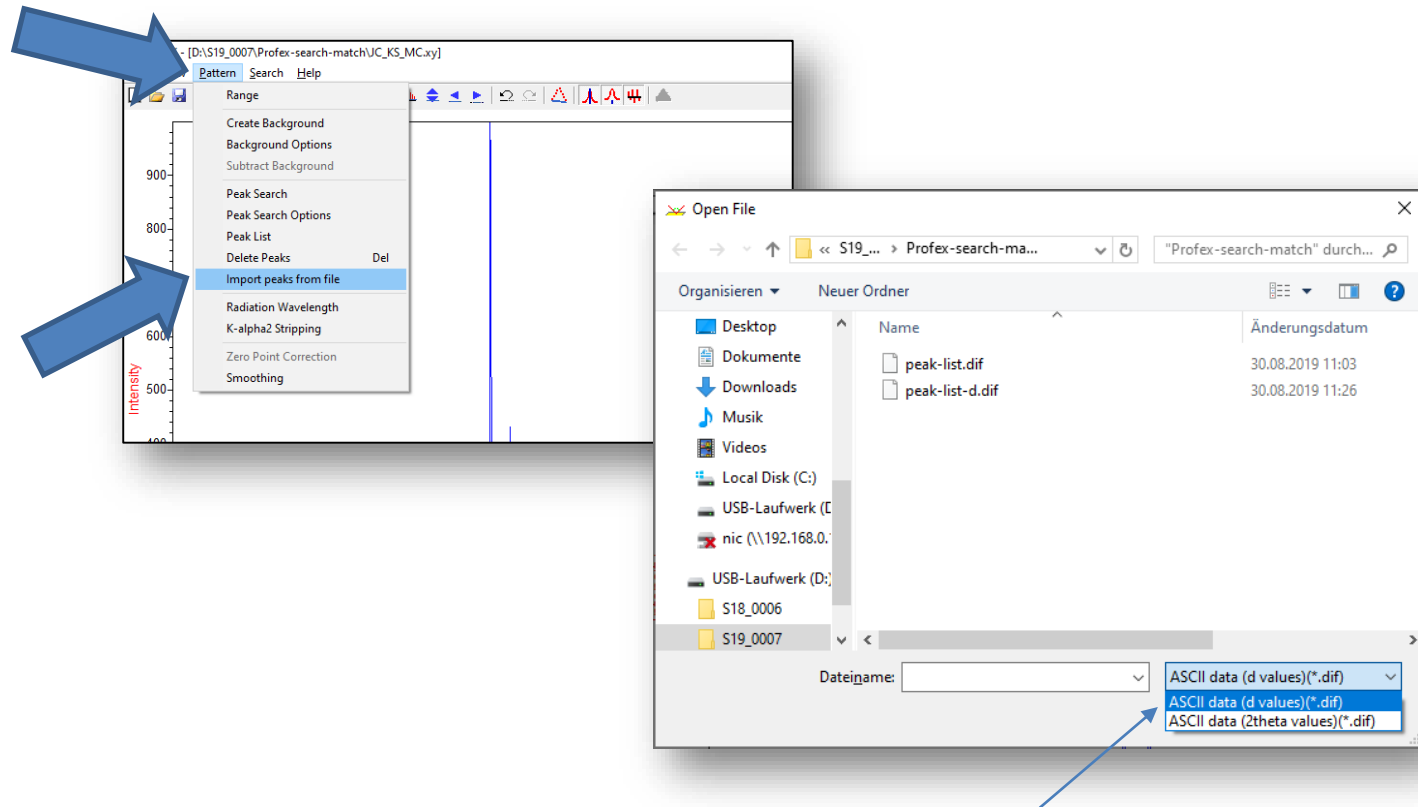
Import Peak List in QualX2

File → Import diffraction data

- Select *.xy file
- Wavelength: CU

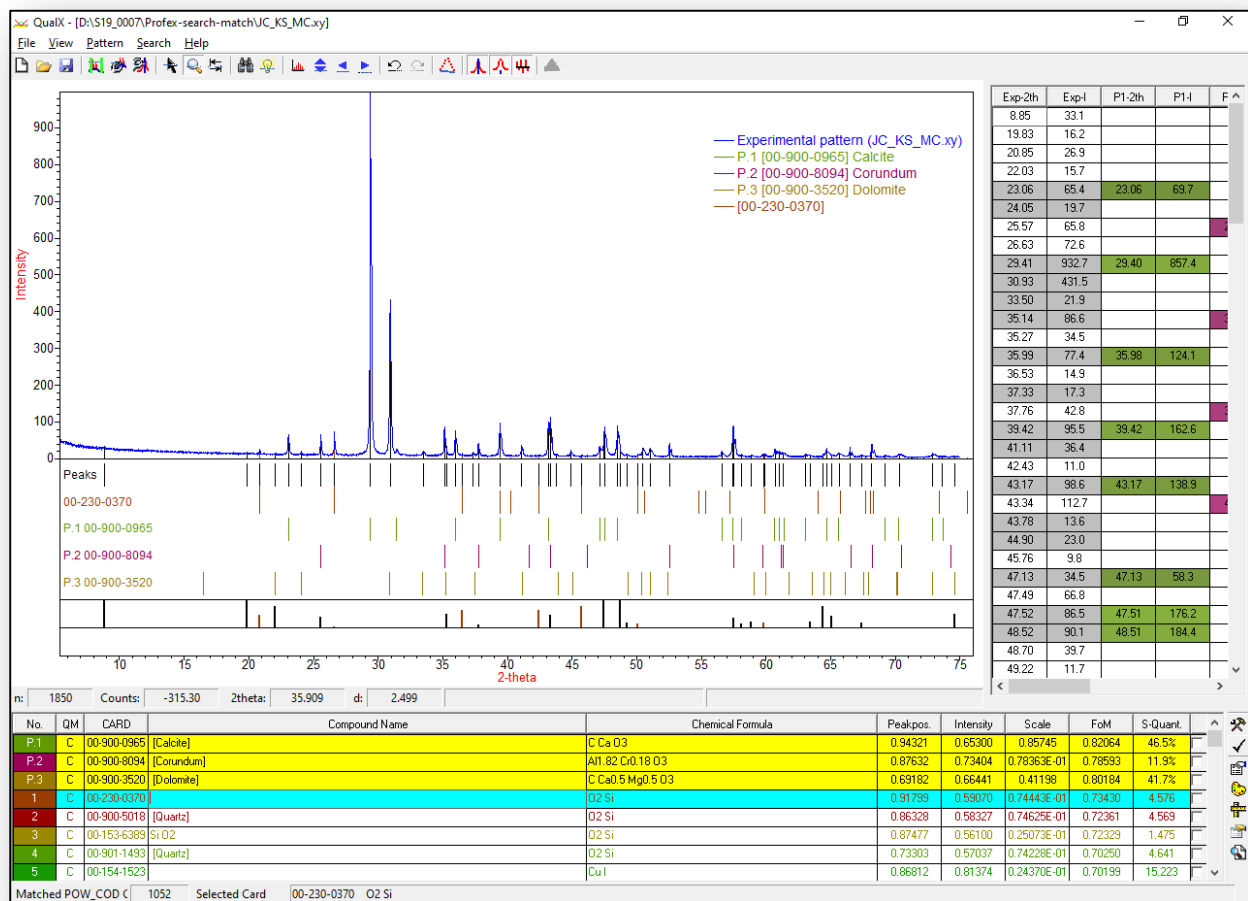


Import Peak List in QualX2



Select format depending on which type of data was exported from Profex.

Import Peak List in QualX2



After lunch:
How to convert structure files from
databases to BGMN *.str format

The screenshot displays the Profex 4.0.0-rc190826 software interface. The main window shows the 'Import Structure Files' dialog, where the file 'Calcite.cif' is selected. The 'STR File' tab is active, showing the generated BGMN STR file content:

```

1 PHASE=Calcite // amcsd_0009873
2 Reference=amcsd_0009873 //
3 Formula=Ca C O3 //
4 SpacegroupNo=167 HermannMauguin=R-32/c Setting=1 UniqueAxis=c Lattice=Trigonal //
5 PARAM=A=0.499100 0.494109*0.504091 PARAM=B=0.499100_0.494109*0.504091
6 PARAM=C=1.706200_1.689138*1.723262 //
7 RP=4 k1=0 k2=0 PARAM=B1=0_0*0.01 GEWICHT=SPHAR4 //
8 GOAL:Calcite=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1) //
9 E=CA Wyckoff=b x=0.000000 y=0.000000 z=0.000000 TDS=0.007969
10 E=C Wyckoff=a x=0.000000 y=0.000000 z=0.250000 TDS=0.007580
11 E=O Wyckoff=e x=0.257300 y=0.000000 z=0.250000 TDS=0.013063

```

The 'Space Group Settings' dialog is also visible, showing the following table:

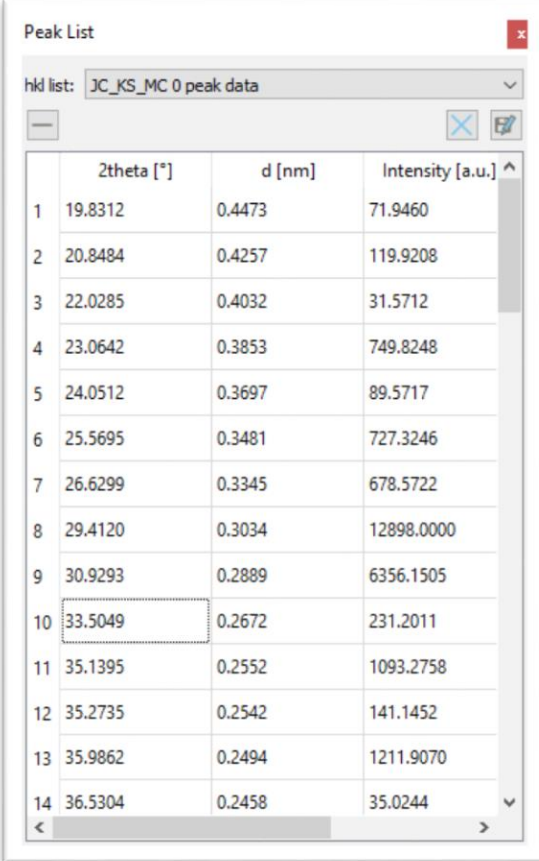
Spacegroup Number	Hermann Mauguin	Wyckoff	Symmetry
161	R-32/c	f (N=36)	x 0 1/4
162	R-32/c	e (N=18)	0 x 1/4
163	R-32/c	d (N=18)	-x -x 1/4
164		c (N=12)	-x 0 3/4
165		b (N=6)	0 -x 3/4
166		a (N=6)	xx 3/4

The 'Import Structure Files' dialog also shows a 'Messages' tab with an 'hkl Plot' graph. The graph displays Intensity (%) on the y-axis (0 to 100) versus Diffraction Angle [° 2θ] on the x-axis (0 to 60). A single sharp peak is visible at approximately 29.5° 2θ, with a density of $\rho = 2.7090 \text{ g/cm}^3$.

Summary:

- Peak detection using EFLECH (part of BGMN)
- Very accurate due to correct wavelength spectrum and instrument configuration
- Export to 3rd party software (tested with Match! And QualX)

- Can be VERY slow (sometimes unable to complete)

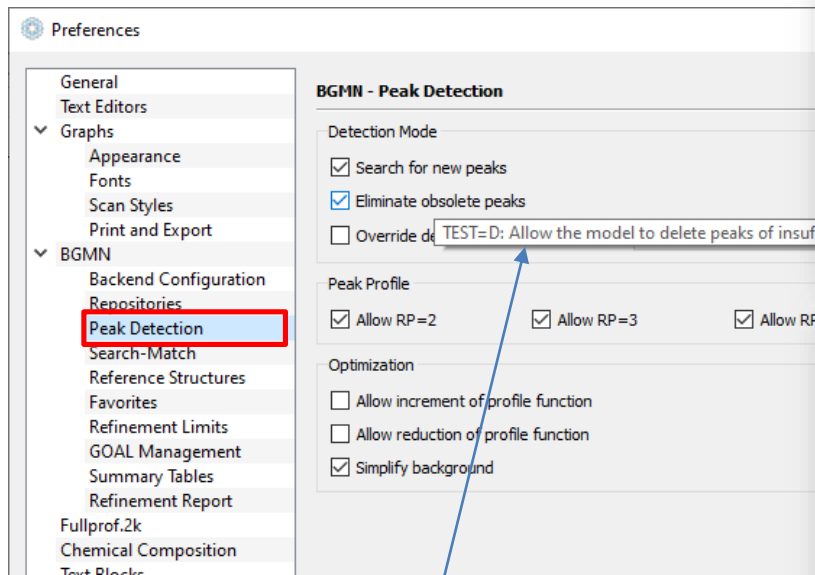


Peak List

hkl list: JC_KS_MC 0 peak data

	2theta [°]	d [nm]	Intensity [a.u.]
1	19.8312	0.4473	71.9460
2	20.8484	0.4257	119.9208
3	22.0285	0.4032	31.5712
4	23.0642	0.3853	749.8248
5	24.0512	0.3697	89.5717
6	25.5695	0.3481	727.3246
7	26.6299	0.3345	678.5722
8	29.4120	0.3034	12898.0000
9	30.9293	0.2889	6356.1505
10	33.5049	0.2672	231.2011
11	35.1395	0.2552	1093.2758
12	35.2735	0.2542	141.1452
13	35.9862	0.2494	1211.9070
14	36.5304	0.2458	35.0244

Tuning peak detection parameters
 Edit → Preferences...



Hover mouse to show tool tip

http://www.bgm.de/eflech_variables.html

EFLECH variables

[Site map](#)

[Up](#) [EFLECH](#) [EFLECH variables](#) [INDEX](#)

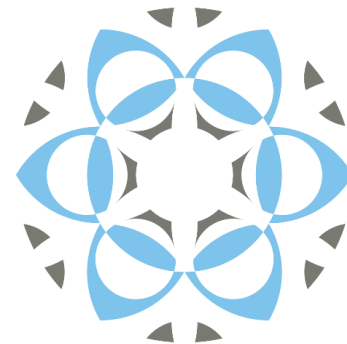
[INDEX variables](#) [Indexing example](#) [Download Page](#)

TEST
 Concatenation of all possible changes, which will performed automatically to reach the output model.
 Default is TEST=ND+-234U, which switches all changes to possible. The letters mean:

- N Search for new peaks.
- D Search for possible deletion of peaks.
- + Search for possible improvement of peaks RP=2->3->4
- Search for possible simplification of peaks RP=4->3->2
- 2 Peaks may change to RP=2 (caused by N or -)
- 3 Peaks may change to RP=3 (caused by N or + or -)
- 4 Peaks may change to RP=4 (caused by N or +)
- U Search for simplification of background

New Features in Profex 4

- GUI changes
- Search / Match
- Peak detection
- Interaction with QualX / Match!



Tomorrow:

- Electron-density maps
- Drawing crystal structures with Vesta / Mercury
- Customizing report layouts