RMS Testing • Research • Consulting

Workshop „Rietveld Refinement with Profex“

Lesson 4: Introduction to Profex - Phase Identification

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RMS Foundation, Switzerland

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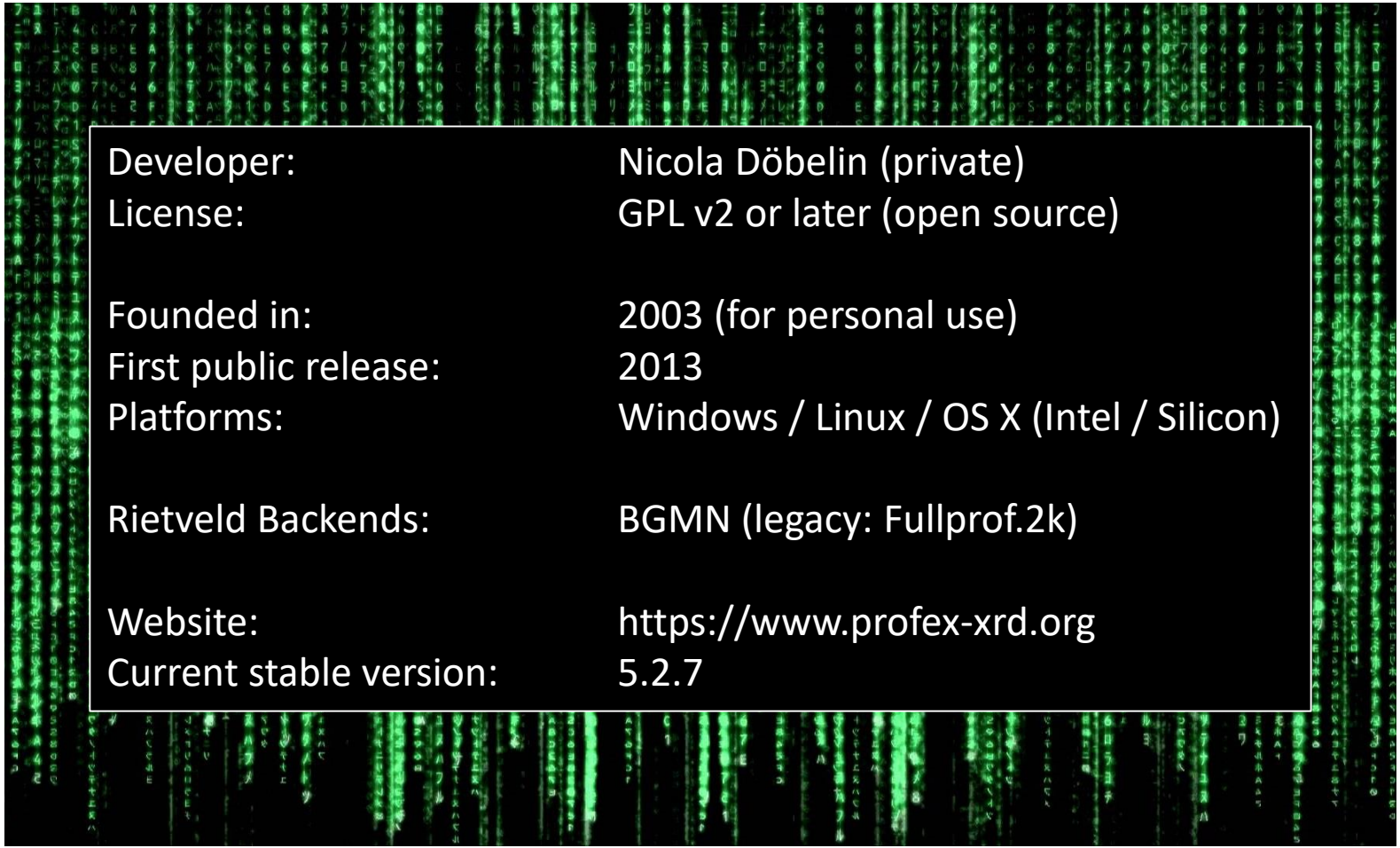
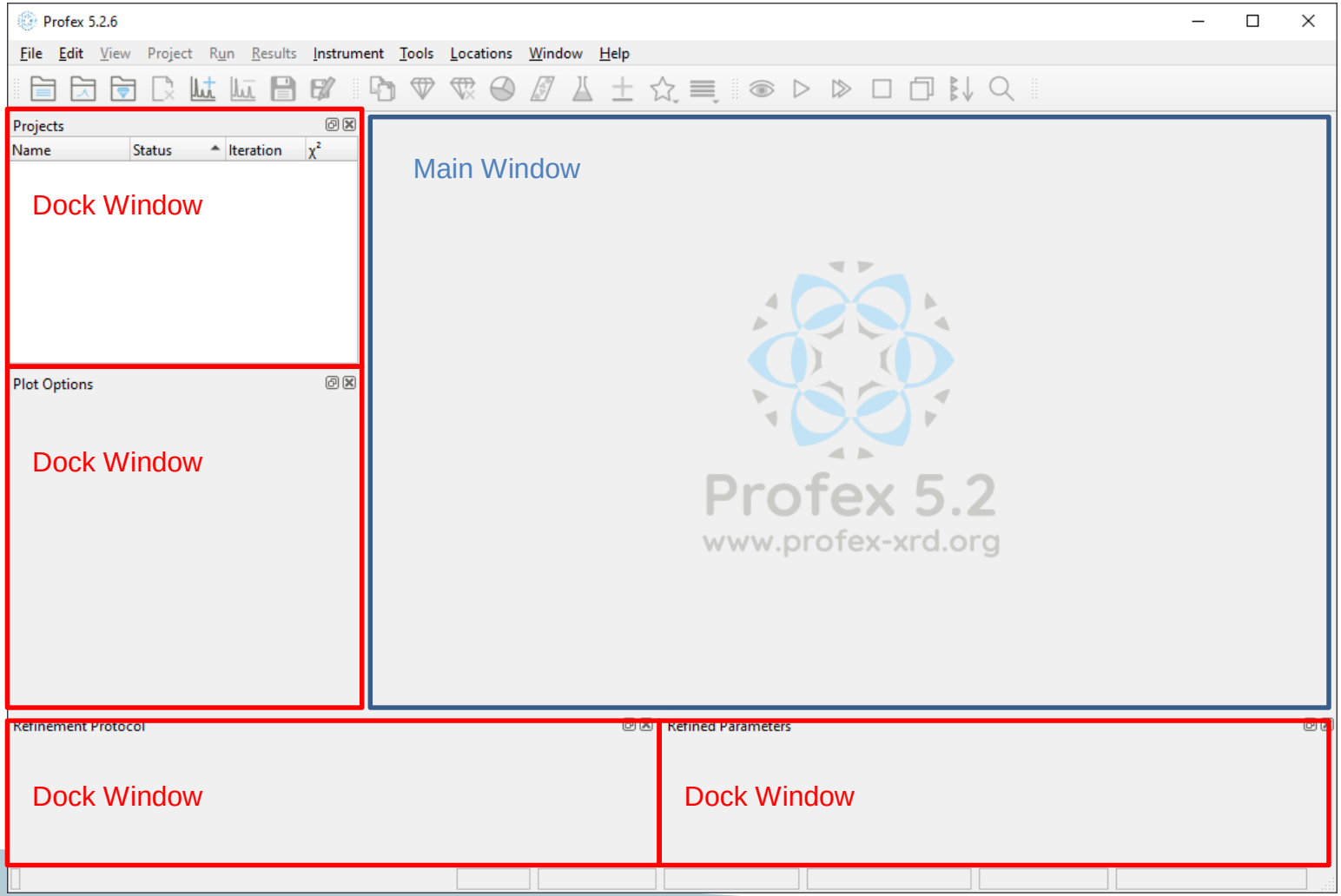
Forschungszentrum Jülich, Germany

Facts about Profex



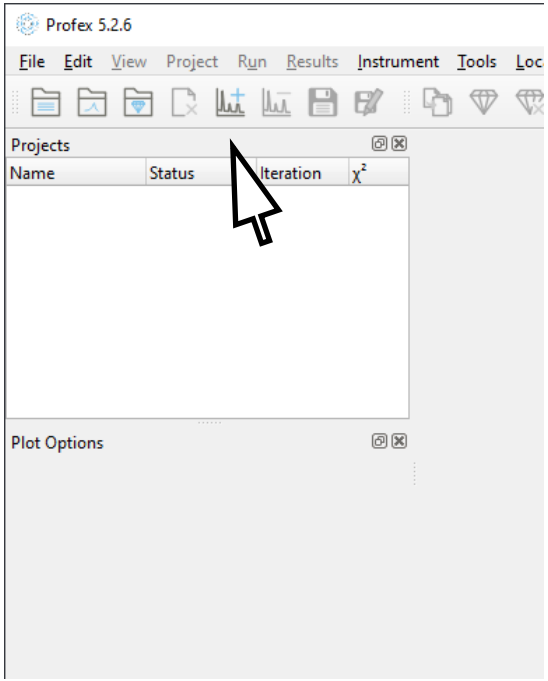
Developer:	Nicola Döbelin (private)
License:	GPL v2 or later (open source)
Founded in:	2003 (for personal use)
First public release:	2013
Platforms:	Windows / Linux / OS X (Intel / Silicon)
Rietveld Backends:	BGMN (legacy: Fullprof.2k)
Website:	https://www.profex-xrd.org
Current stable version:	5.2.7

Profex User Interface

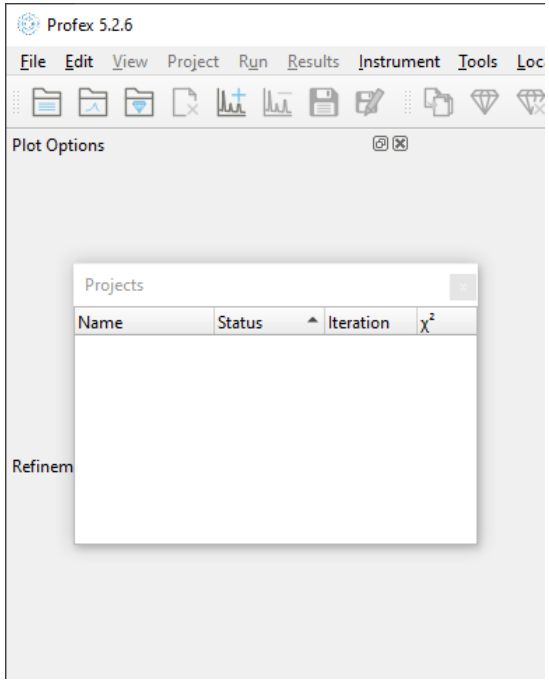


Profex User Interface

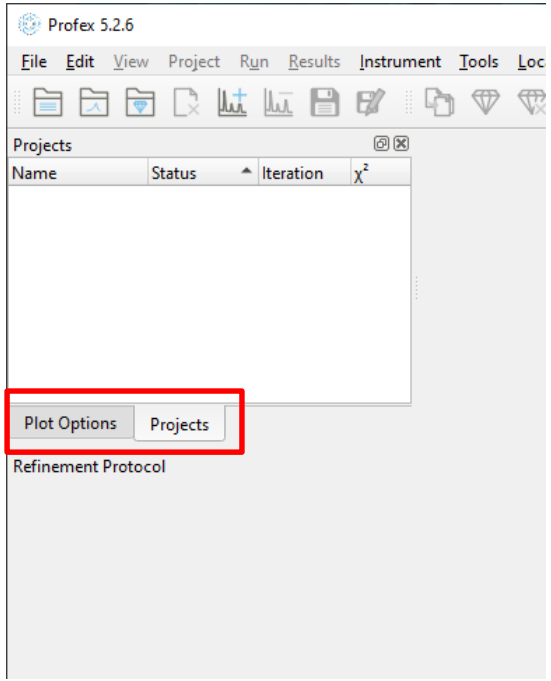
Docked



Floating

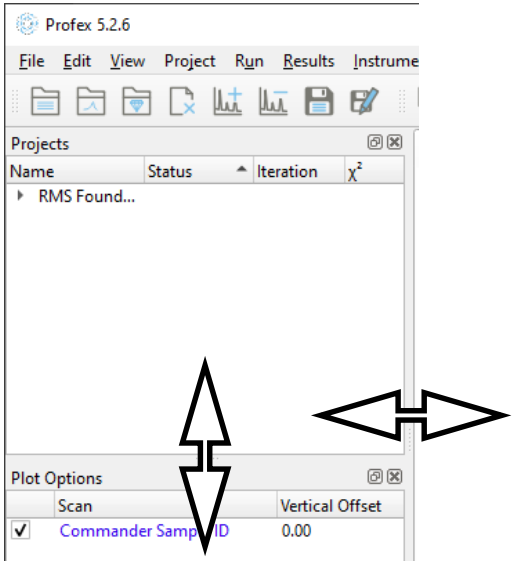


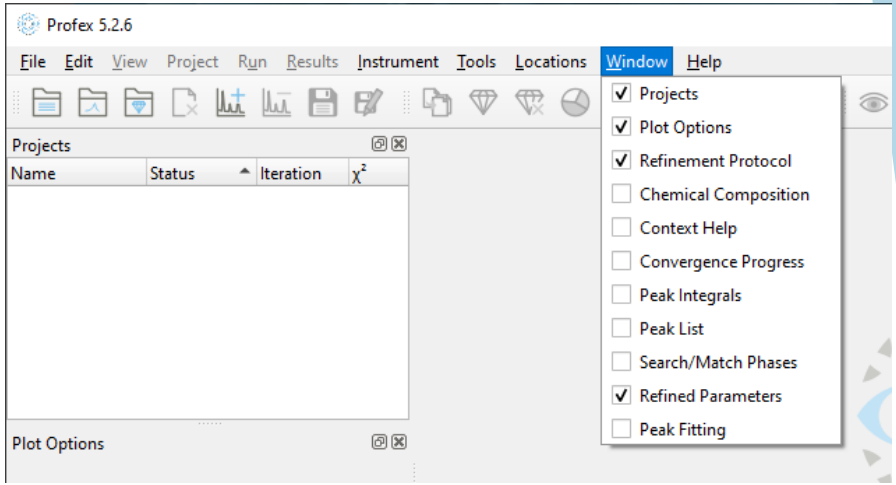
Stacked



To re-arrange:
Grab title bar of dock windows with the mouse and drag.

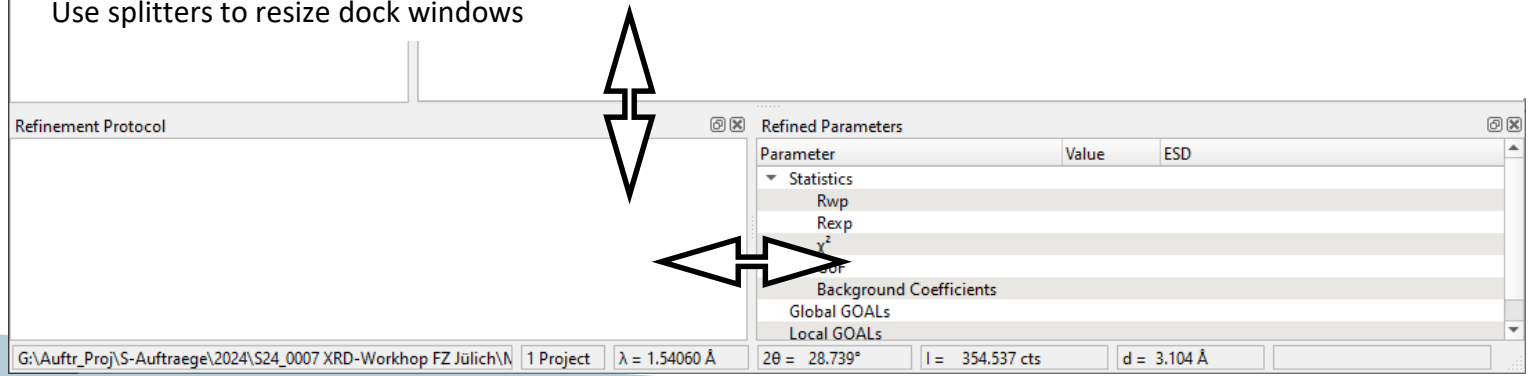
Profex User Interface



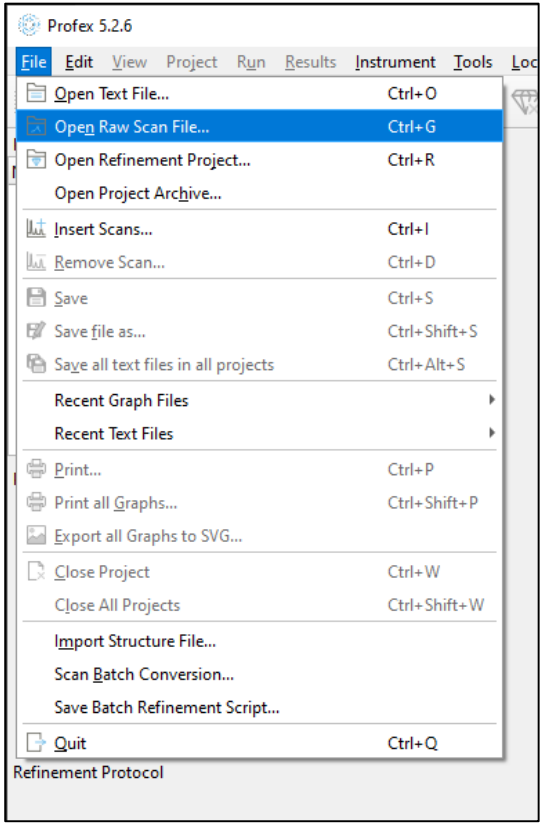


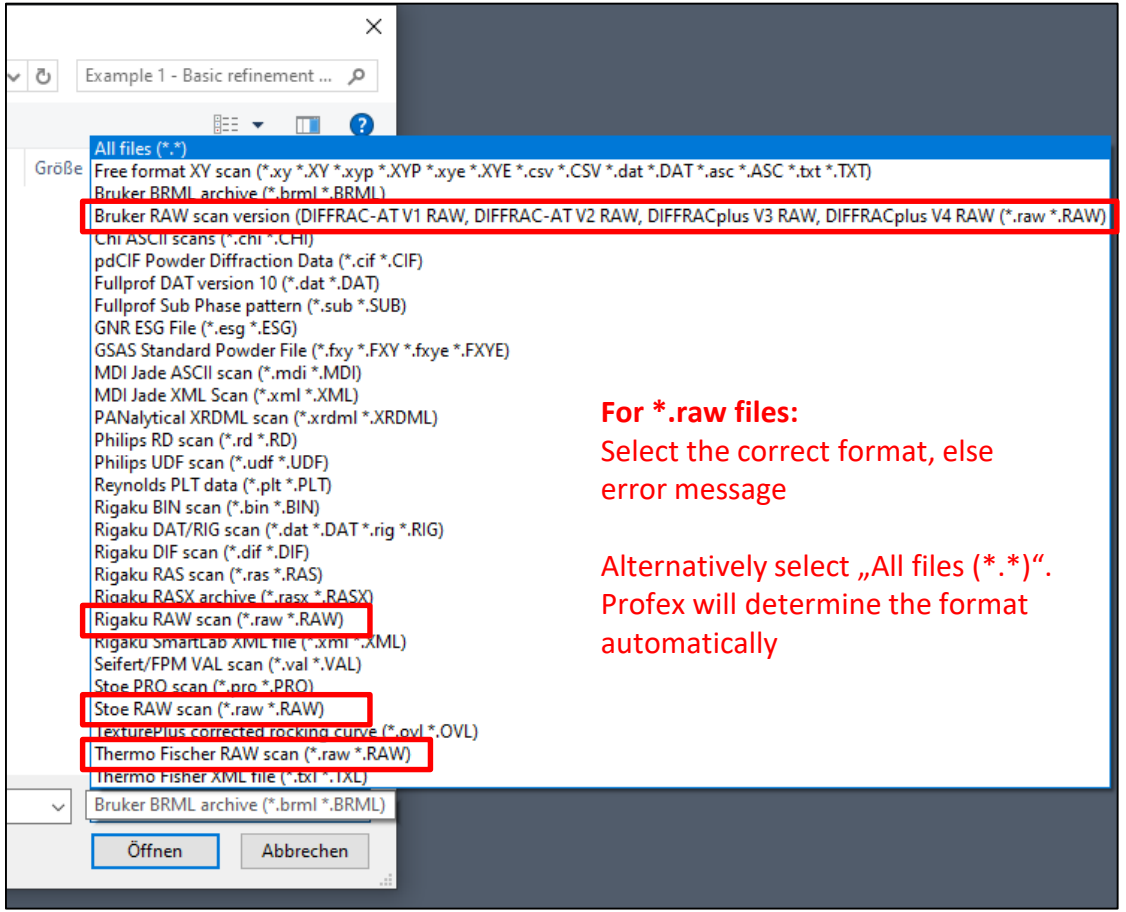
Closed dock windows can be opened from the „Window“ menu

Use splitters to resize dock windows



Loading Scan Files





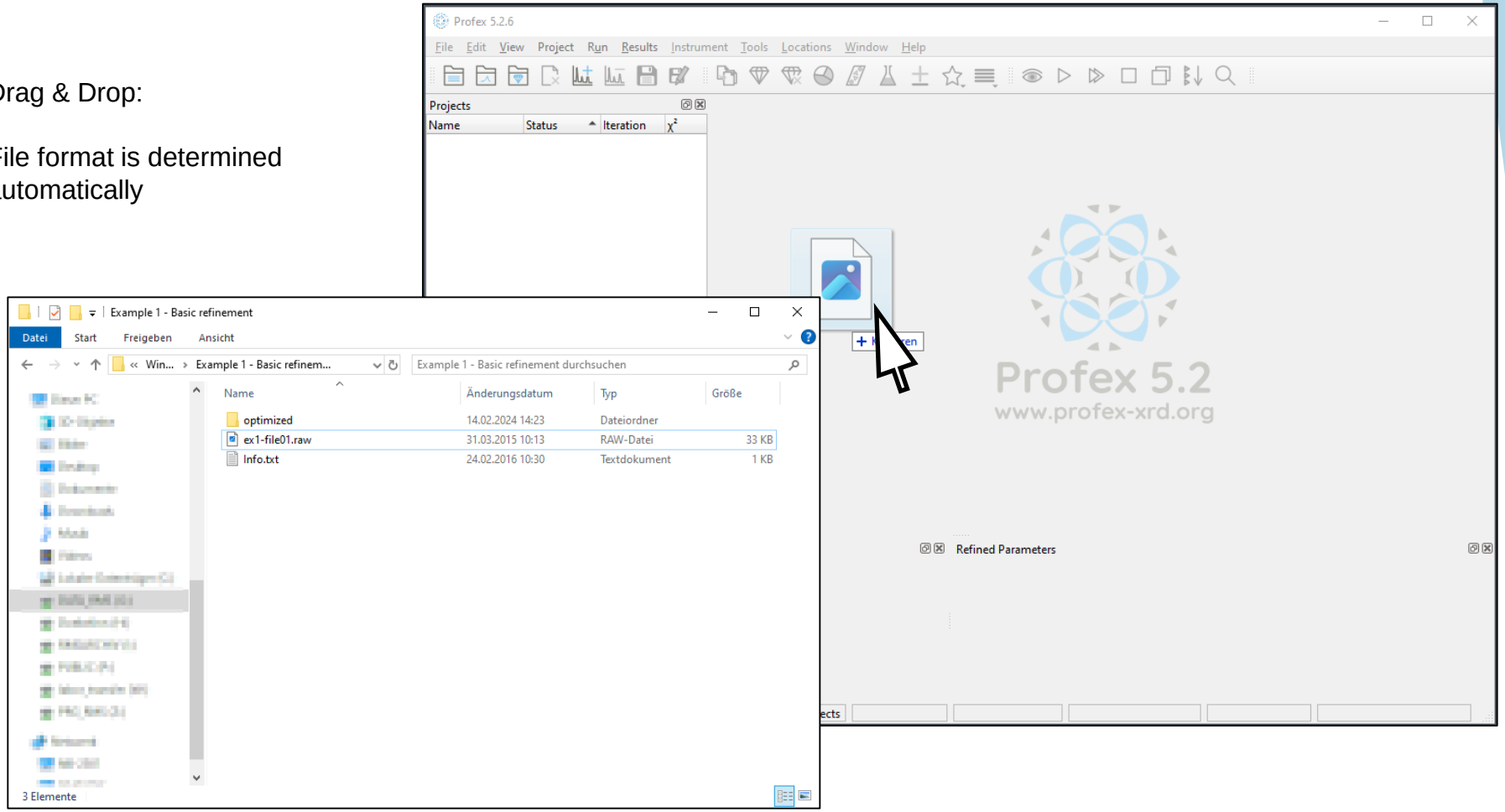
For *.raw files:
Select the correct format, else error message

Alternatively select „All files (*.*)“. Profex will determine the format automatically

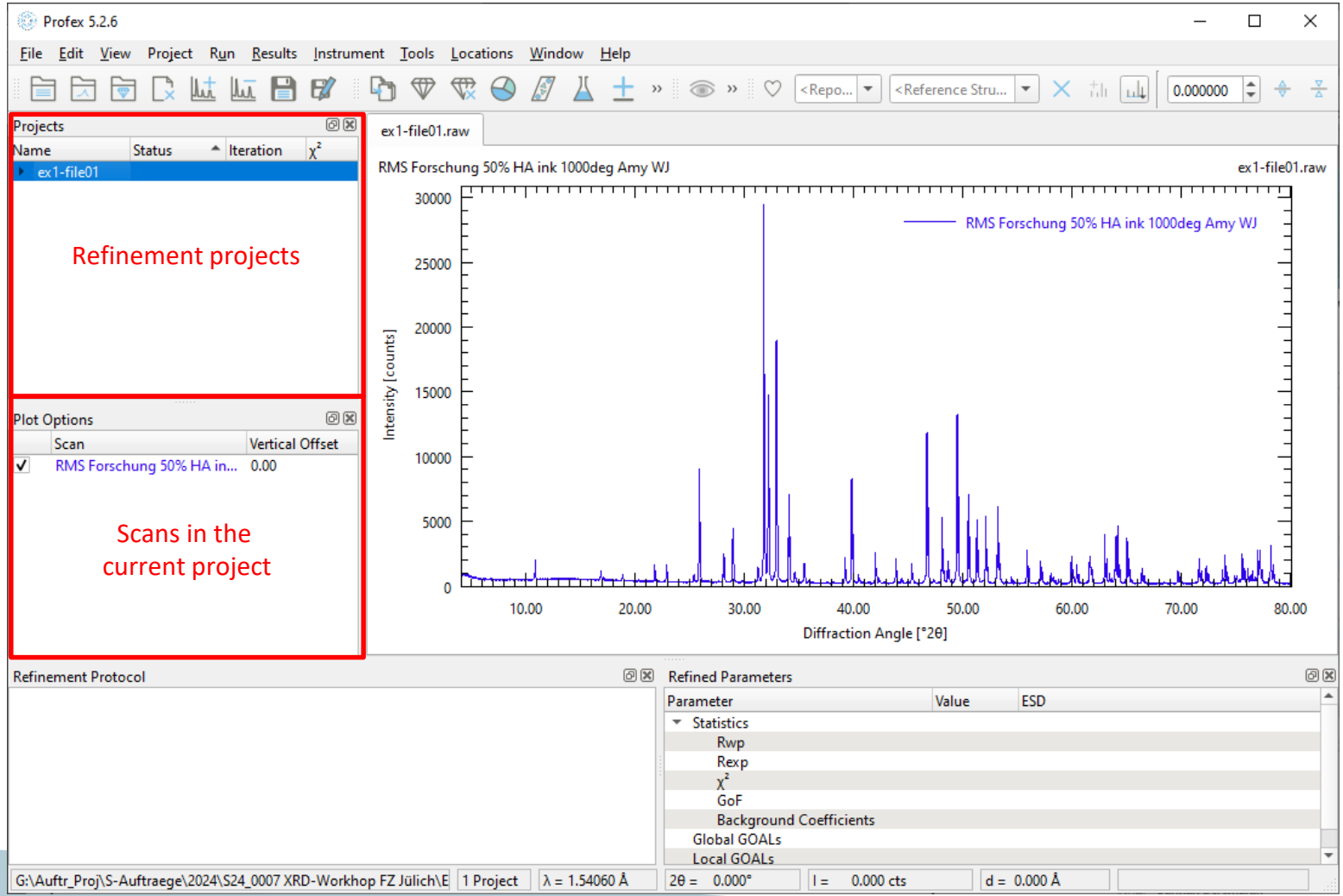
Loading Scan Files

Drag & Drop:

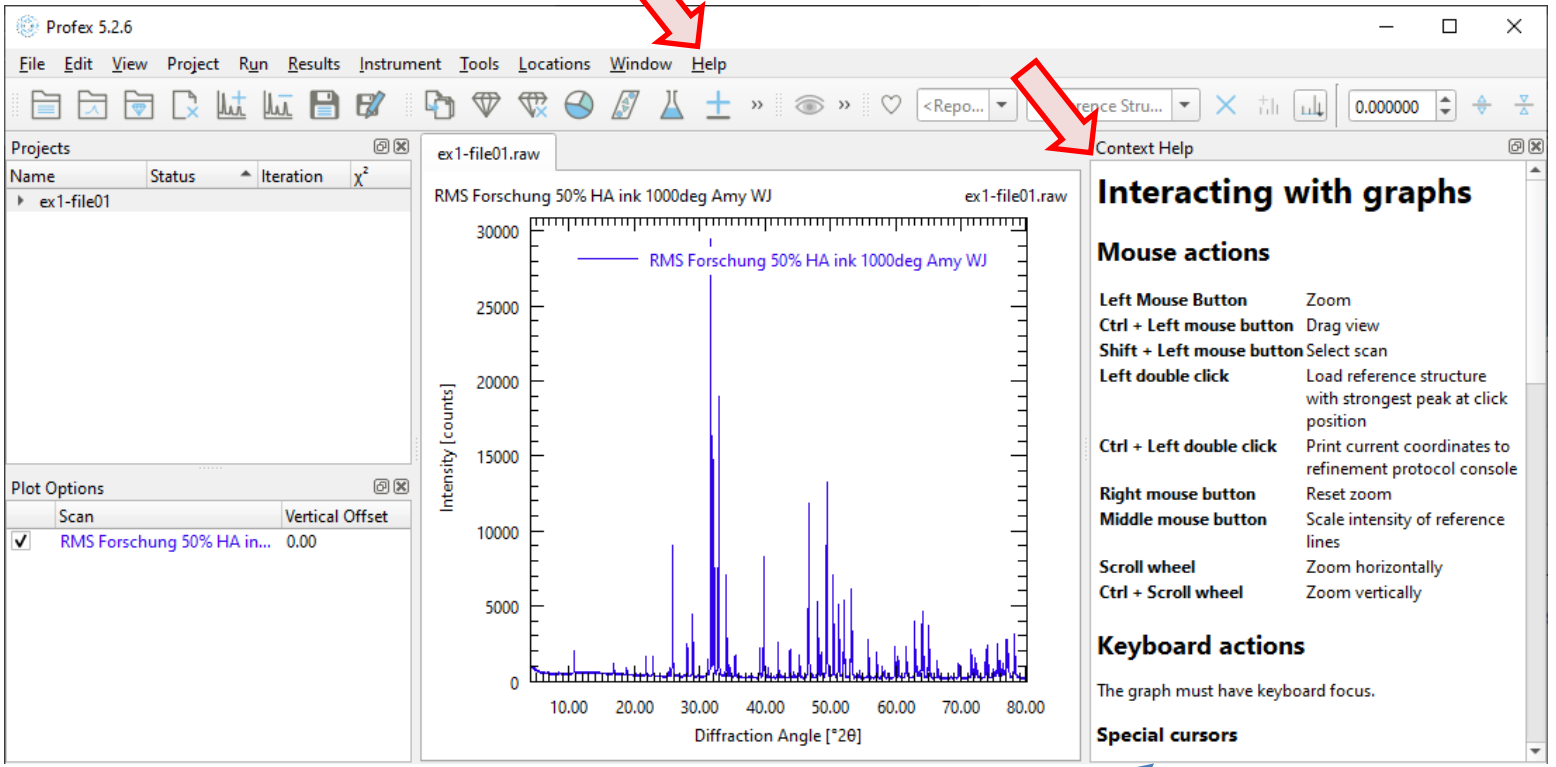
File format is determined automatically



Loading Scan Files



Loading Scan Files



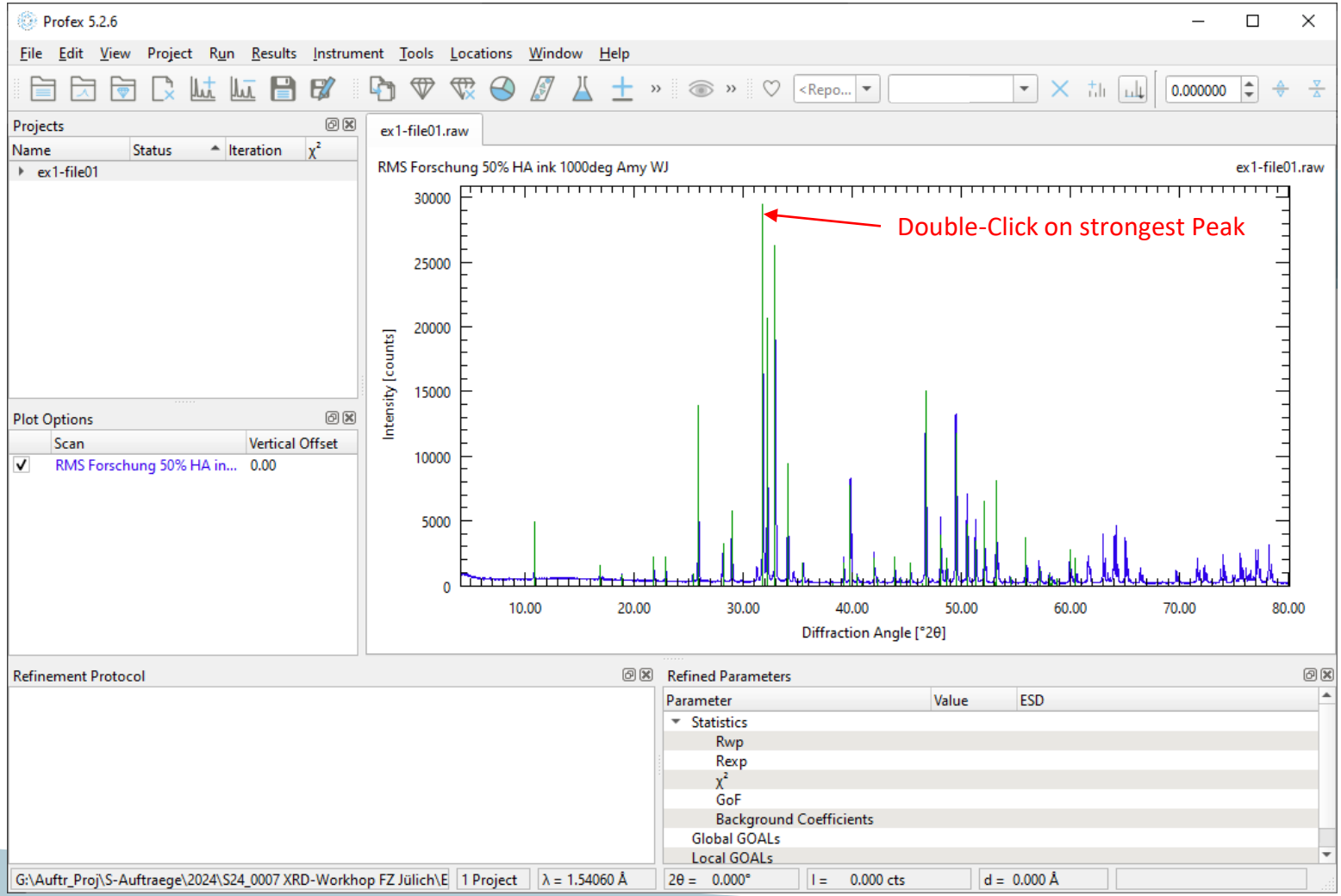
„Help → Mouse and Keyboard commands“

Phase Identification

3 Different approaches to phase identification in Profex

- 1: Double-click strongest peak
  - + Fast
  - - Can be unreliable
  - - Only searches internal database (~1000 phases)
- 2: Run full-pattern search-match in Profex
  - - Slow
  - + Reliable
  - - Only searches internal database (~1000 phases)
- 3: Run peak detection in Profex, import peak list to other search-match software
  - Can be slow
  - Requires other software
  - Searches COD or ICDD database (> 400‘000 phases)

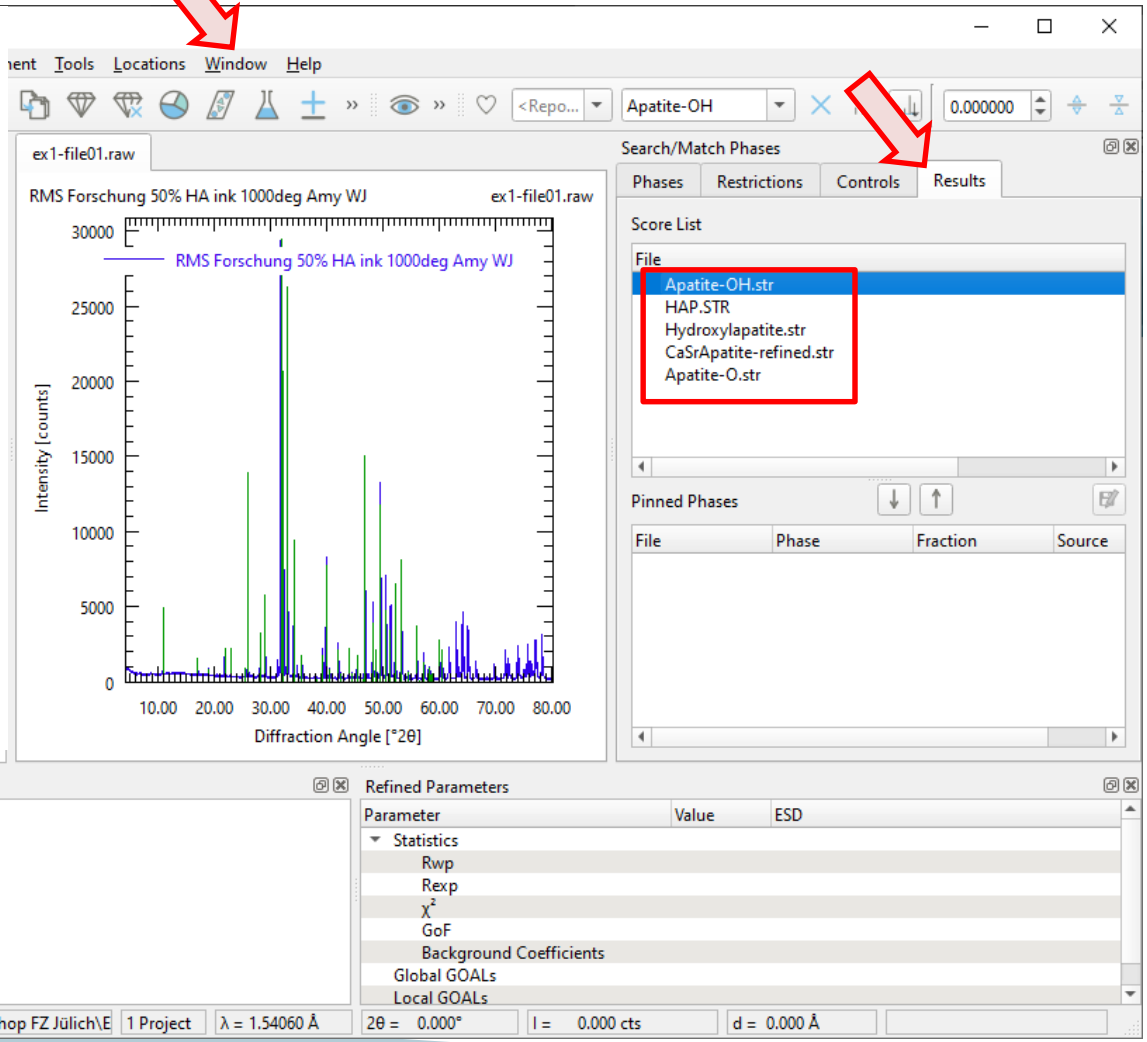
Phase Identification: Double Click on Strongest Peak



Phase Identification: Double Click on Strongest Peak

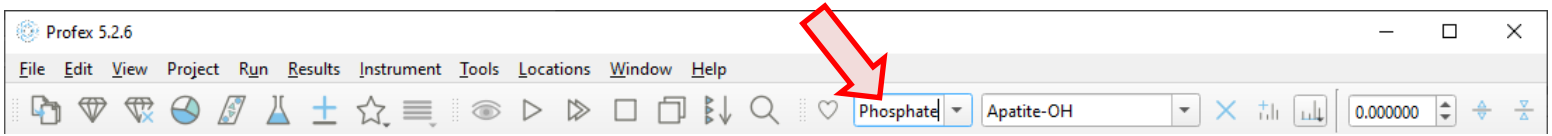
Best matching phases are also shown in Search-Match module:

Window
→ Search/Match Phases
→ Results



Phase Identification: Double Click on Strongest Peak

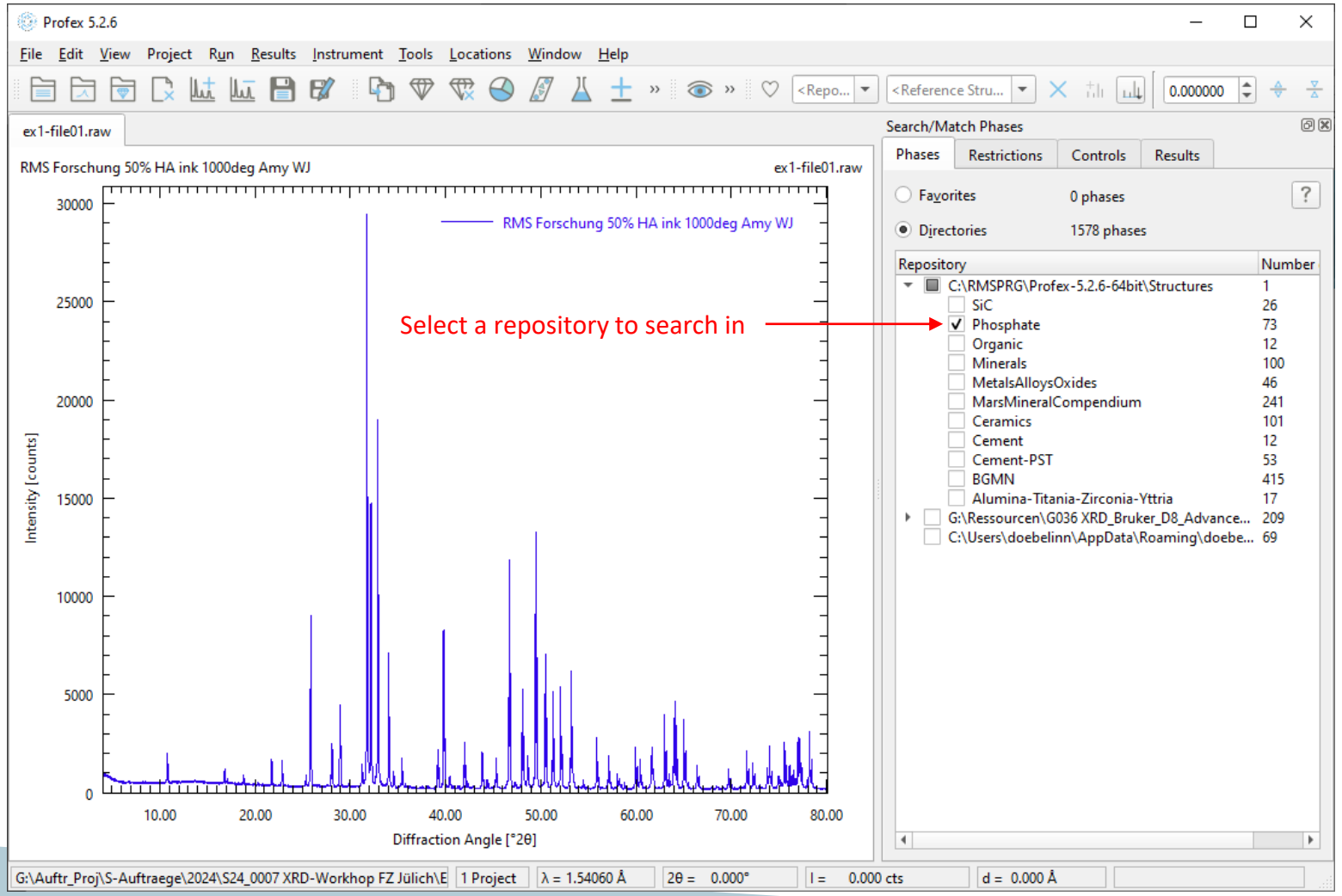
Limit the search to a sub-directory to improve the hit rate



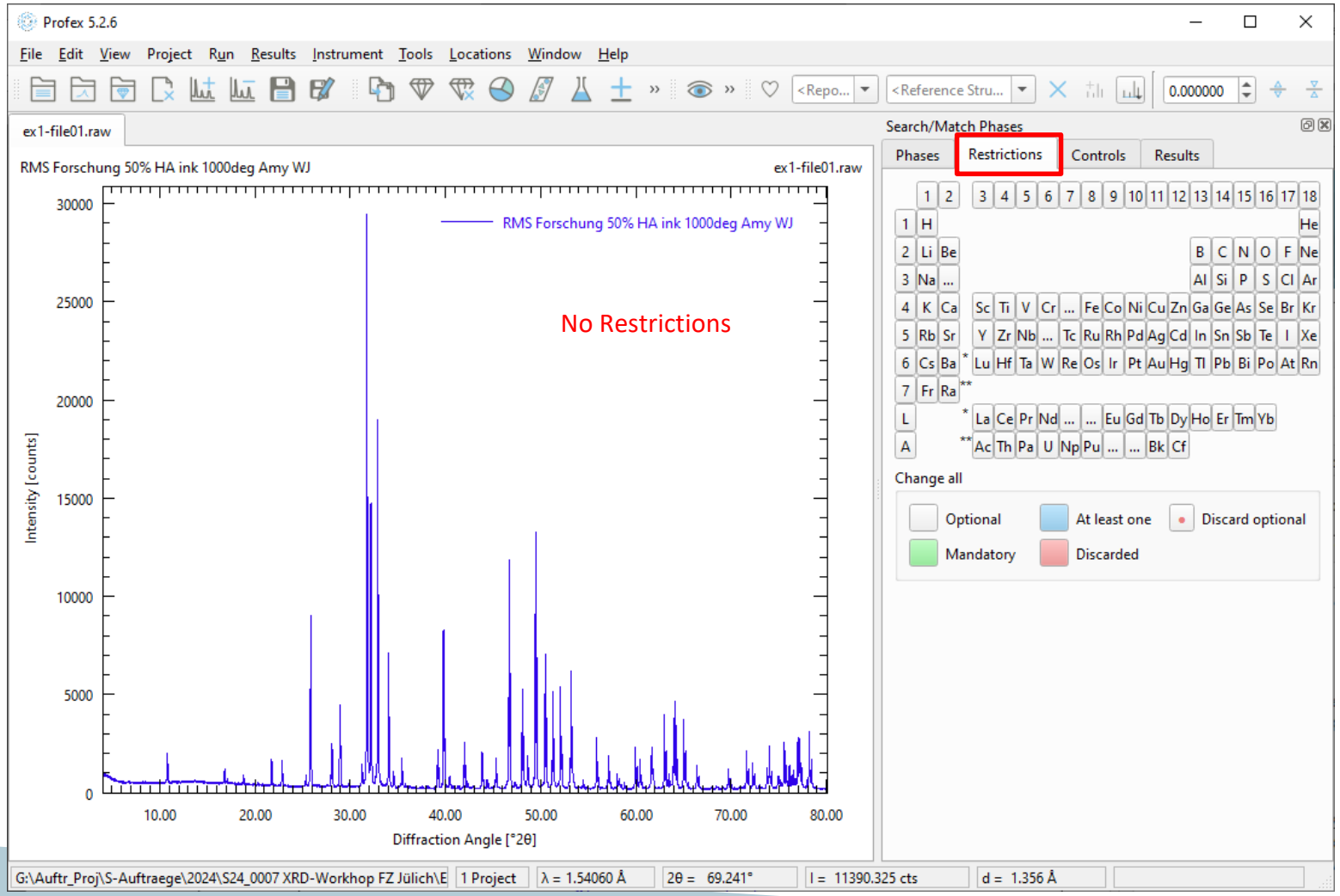
Double-click phase identification is often good enough
to identify the strongest phase.

If not: Use Search/Match Module (Window → Search/Match Phases)

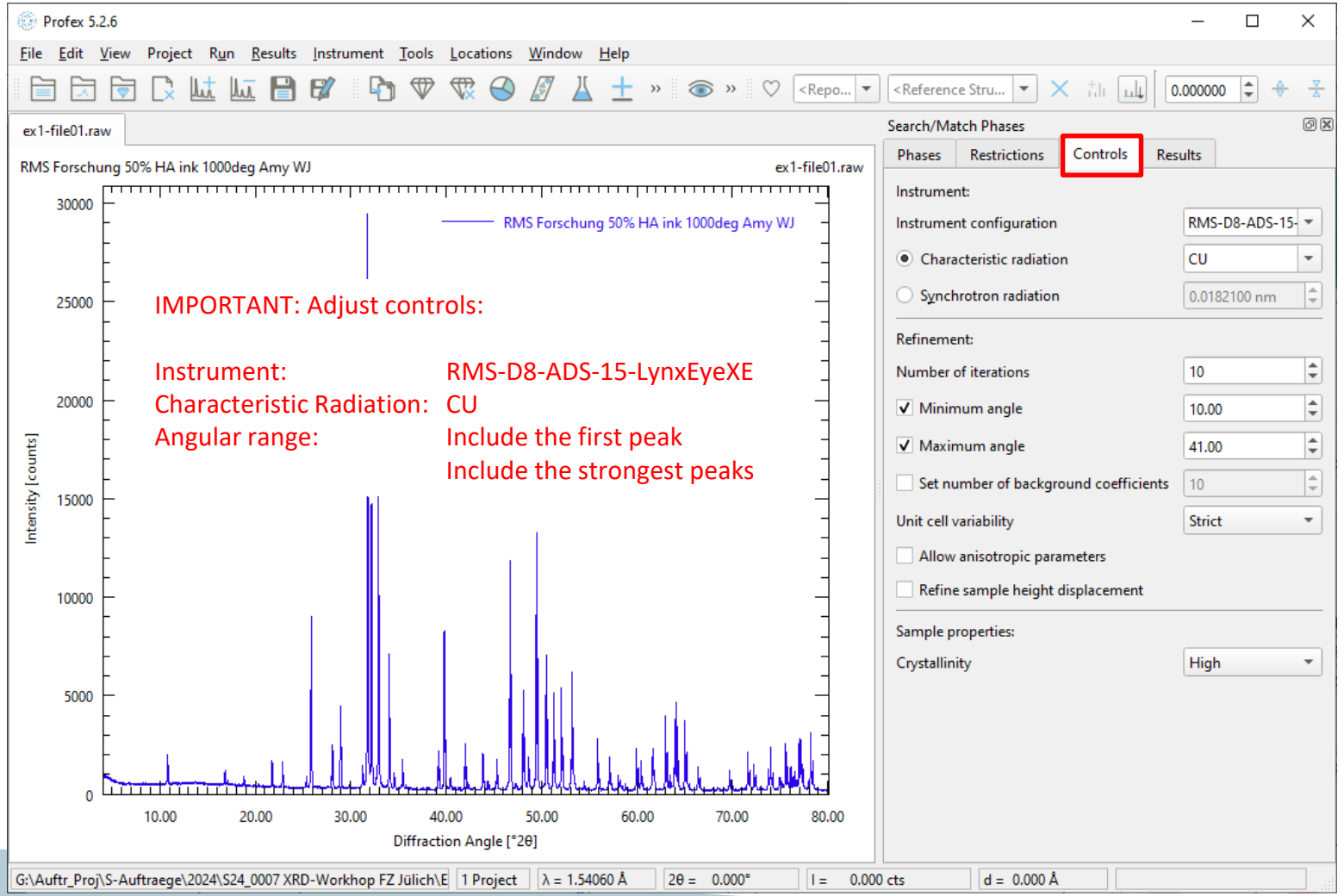
Full-Pattern Search/Match Module



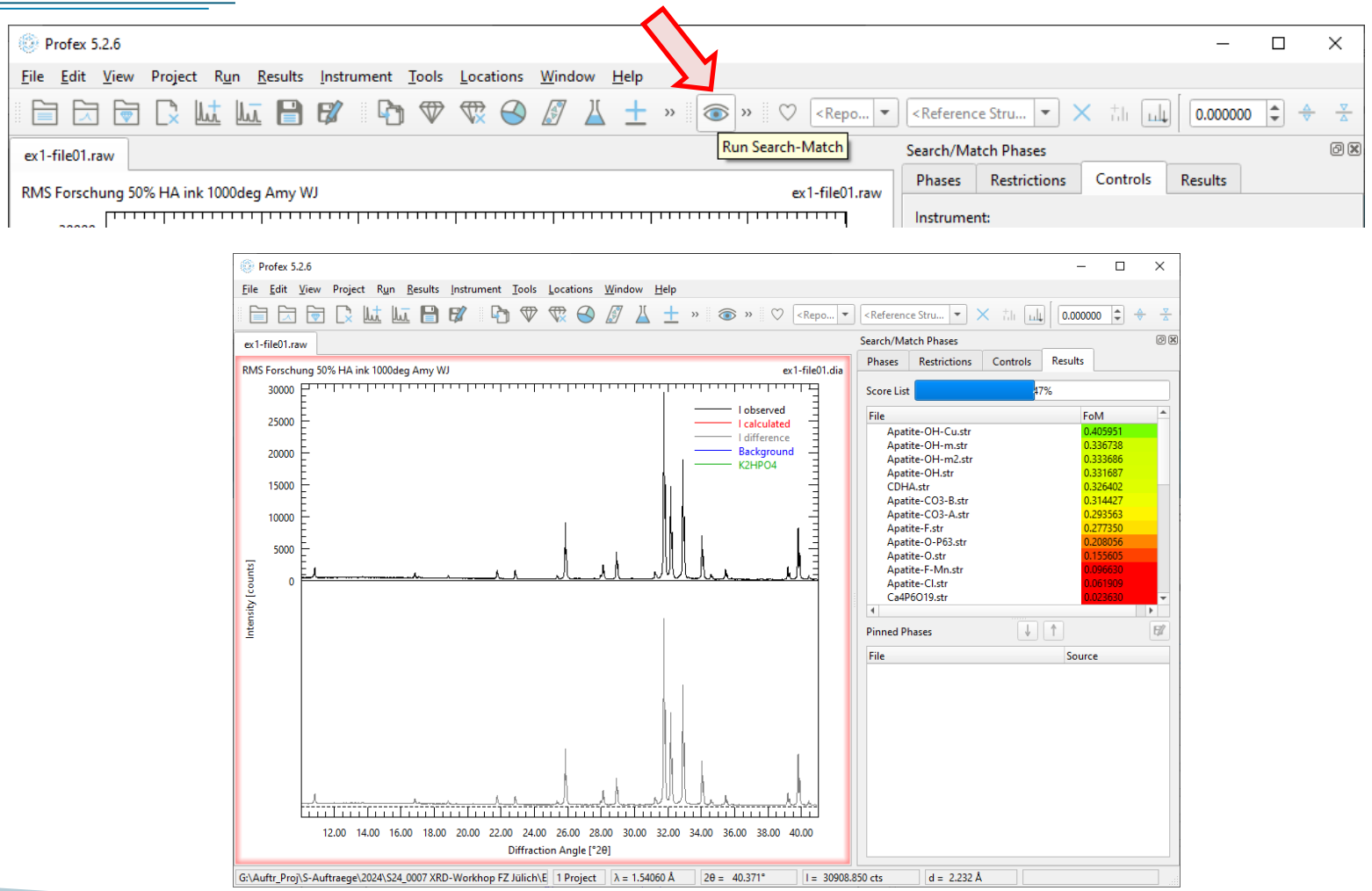
Full-Pattern Search/Match Module



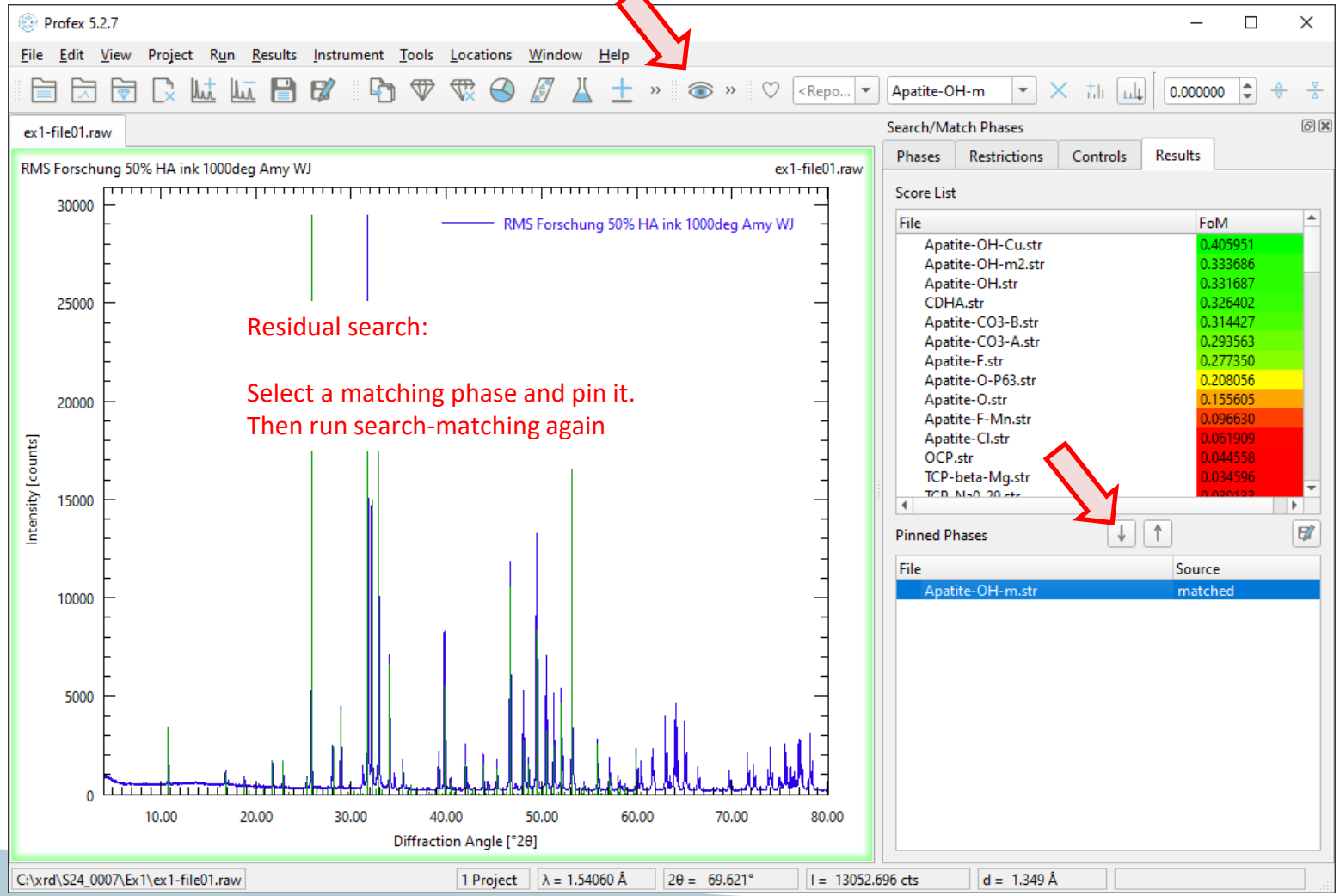
Full-Pattern Search/Match Module



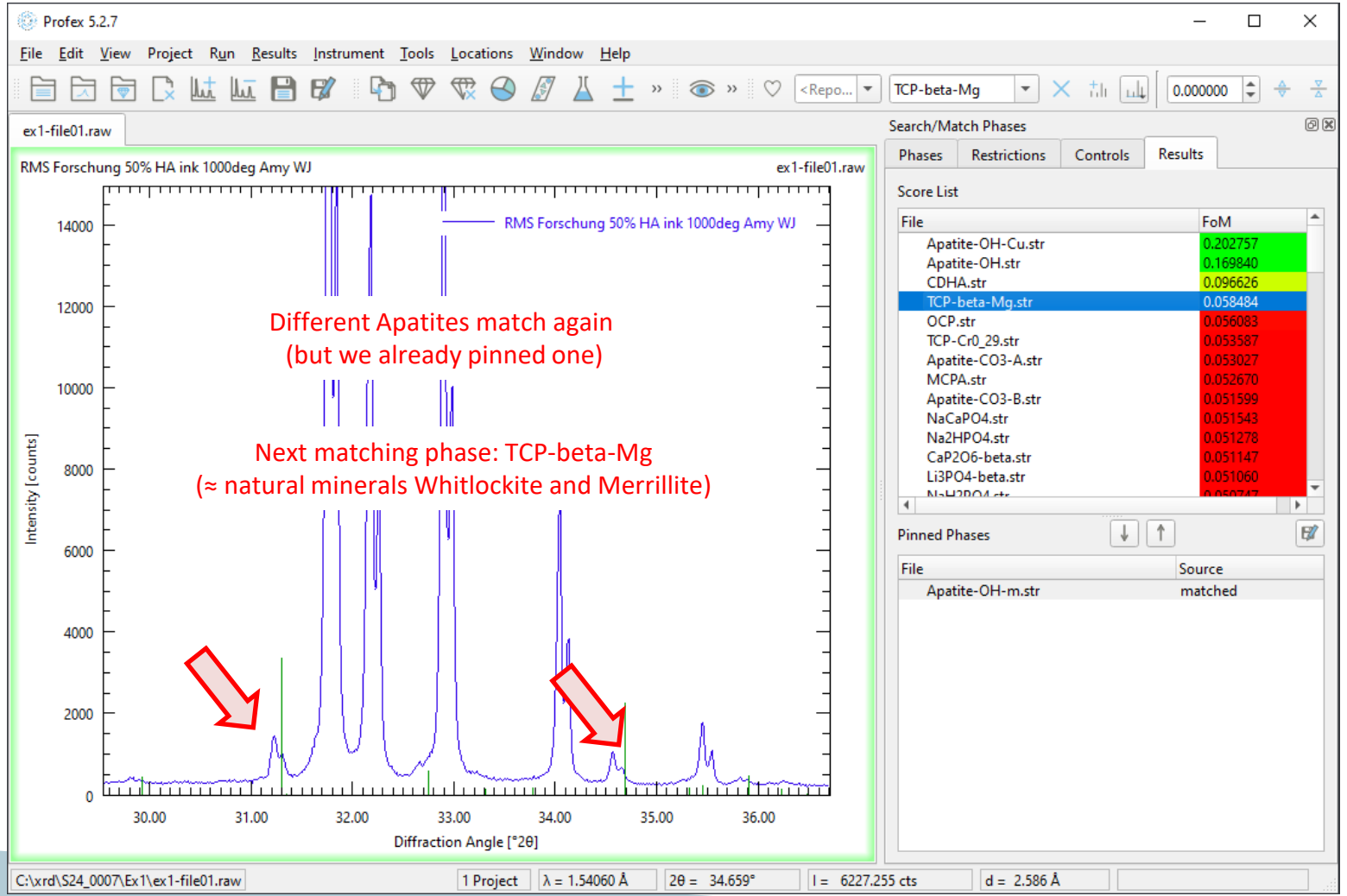
Full-Pattern Search/Match Module



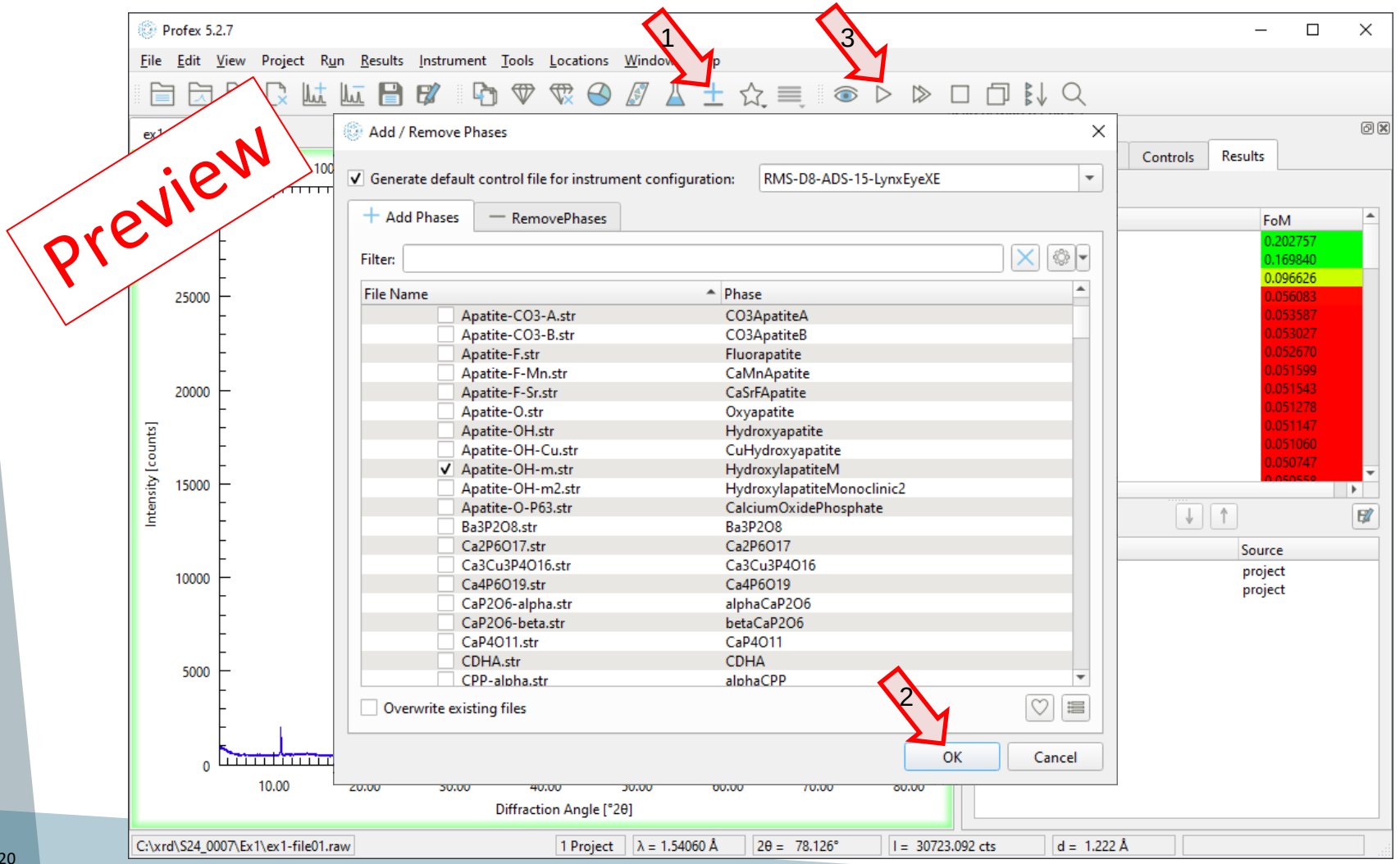
Full-Pattern Search/Match Module



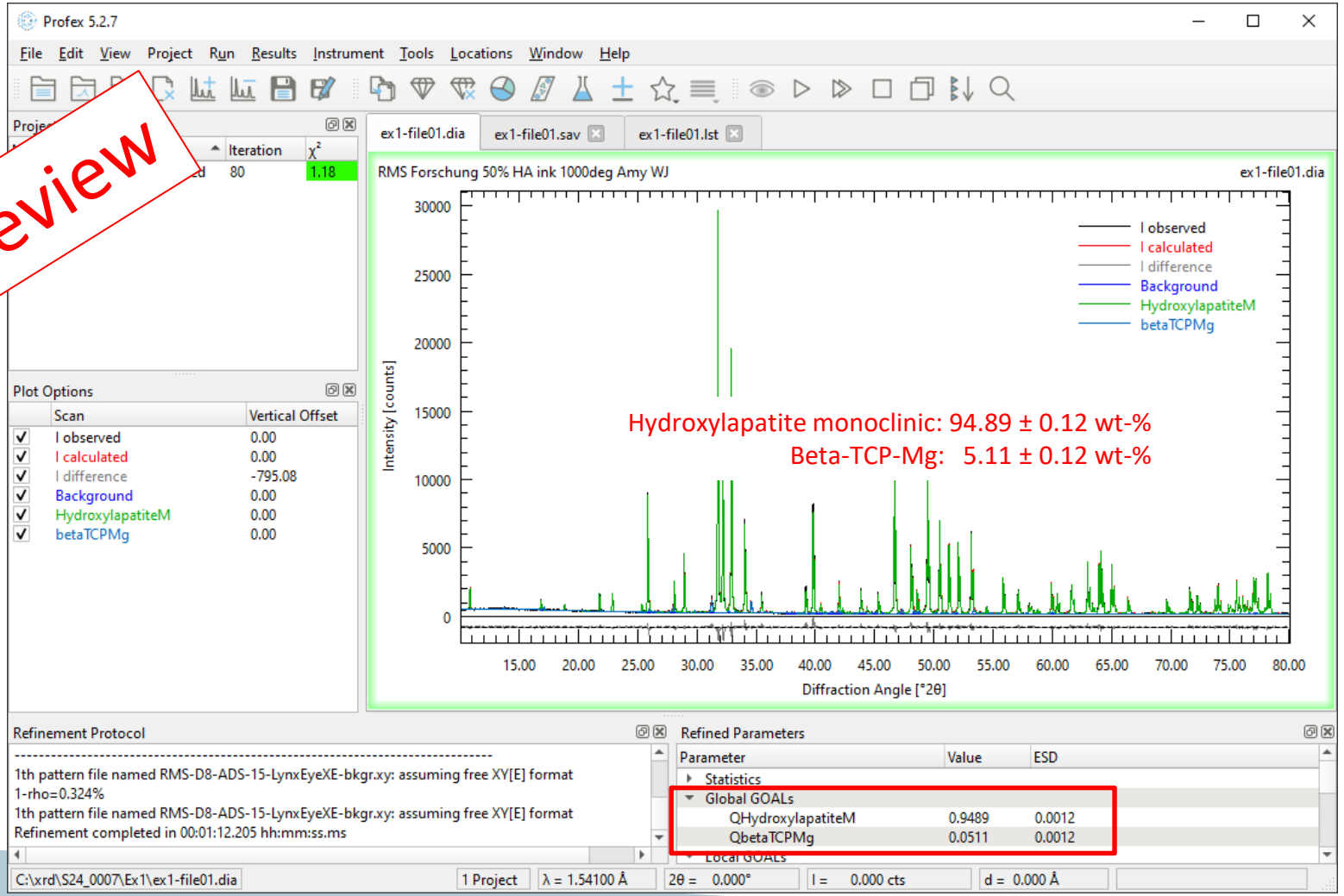
Full-Pattern Search/Match Module



Preview: Create Rietveld Refinement Project



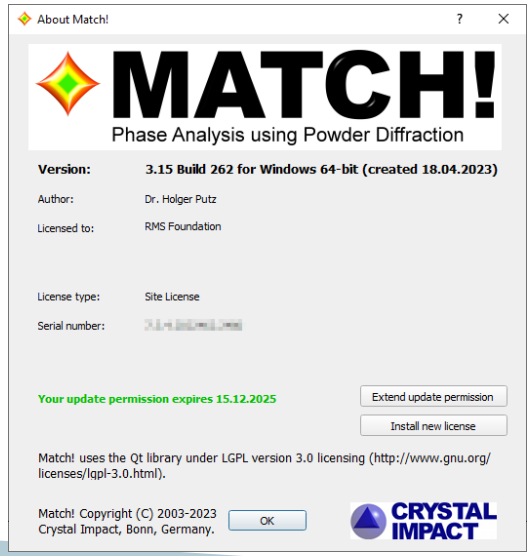
Preview: Rietveld Refinement



Search-Match with 3rd Party Software

Use 3rd-party search/match software to search in large databases:

1. Run peak detection in Profex
   (extremely reliable, but slow)
2. Export peak list
3. Import peak list in 3rd-party software
4. Run search/match on large database

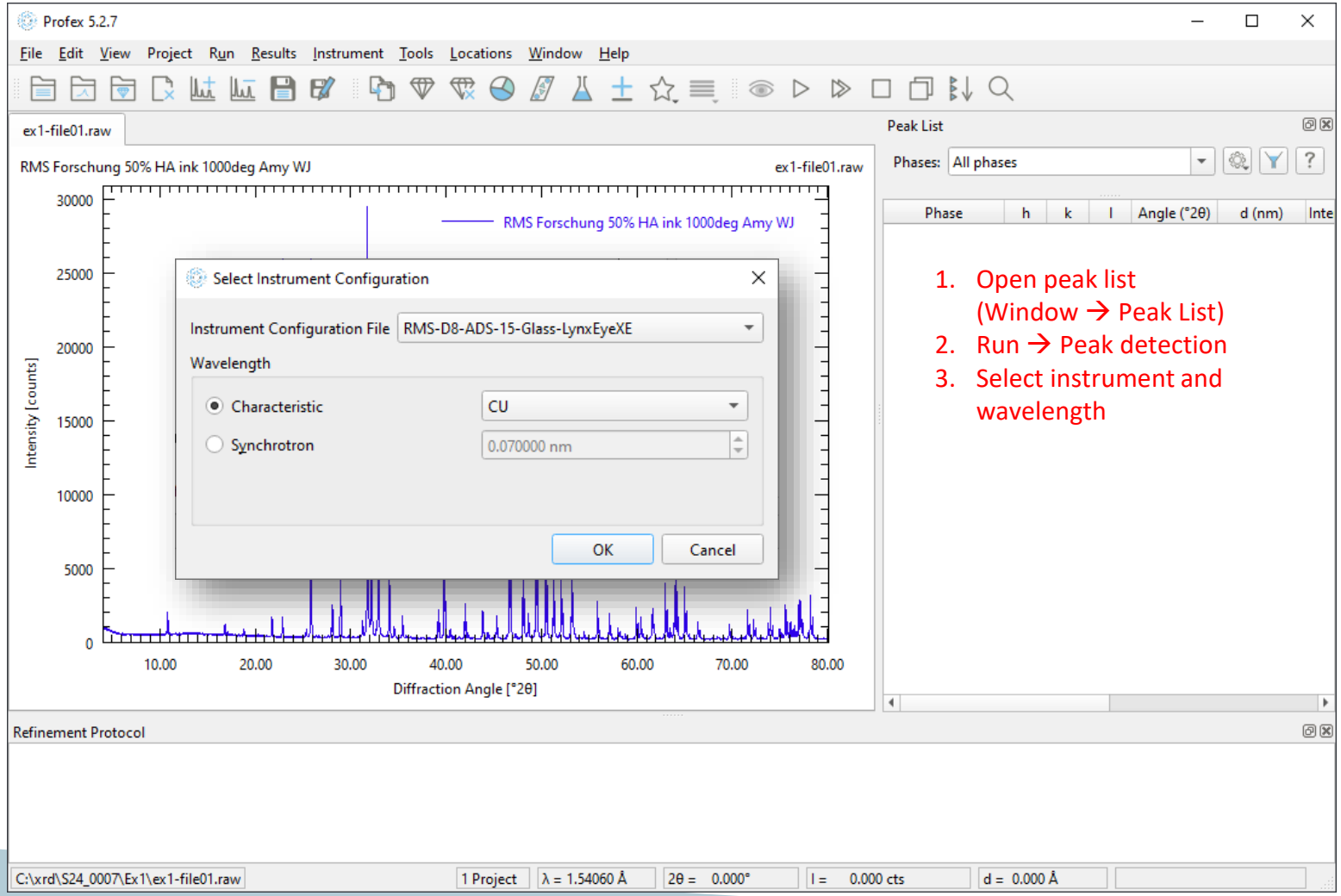


2 different Structure Databases

Crystallography Open Database (COD)
http://www.crystallography.net/cod
Open access

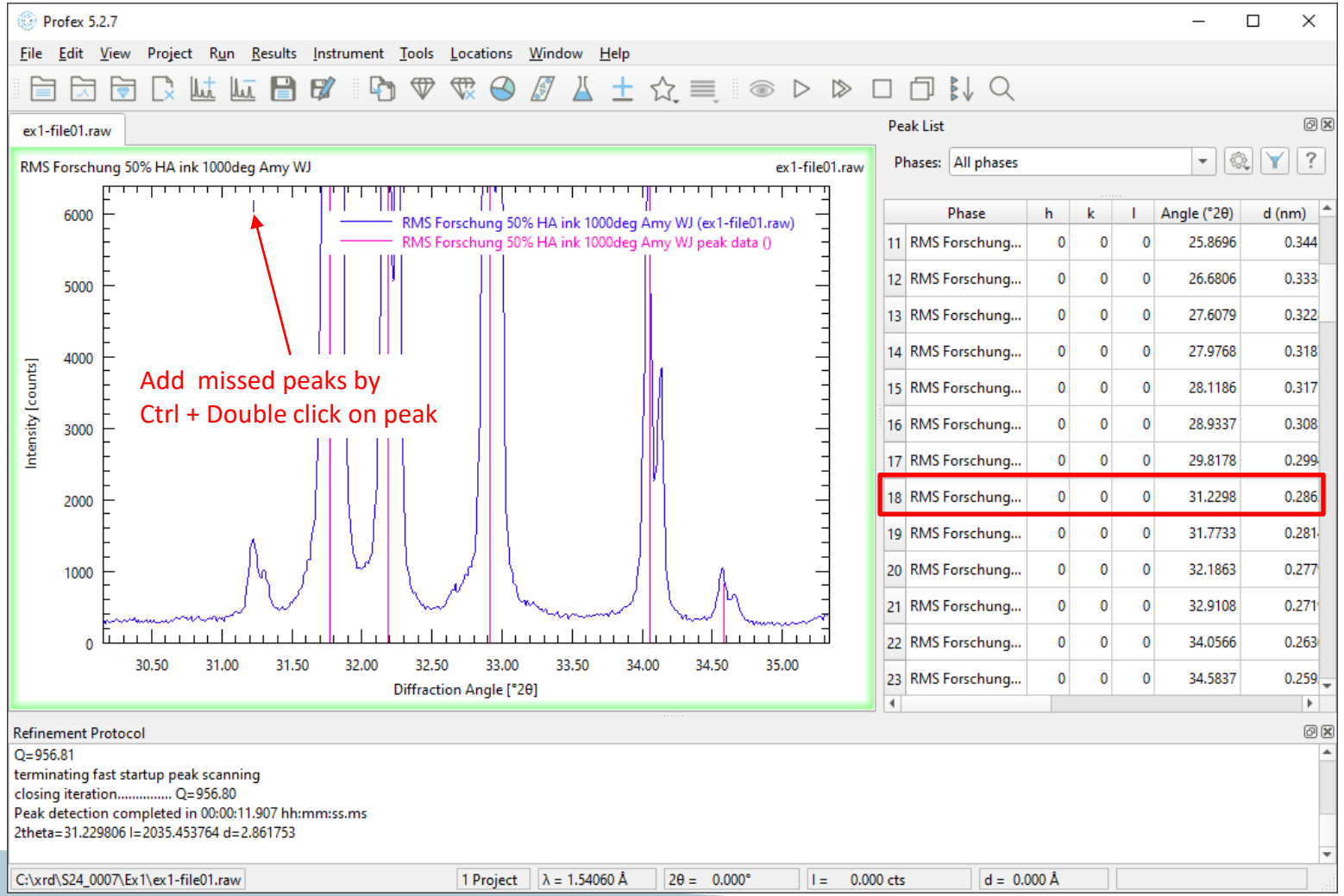
ICDD PDF-4+
https://www.icdd.com/pdf-4-minerals/
Commercial

Peak Detection

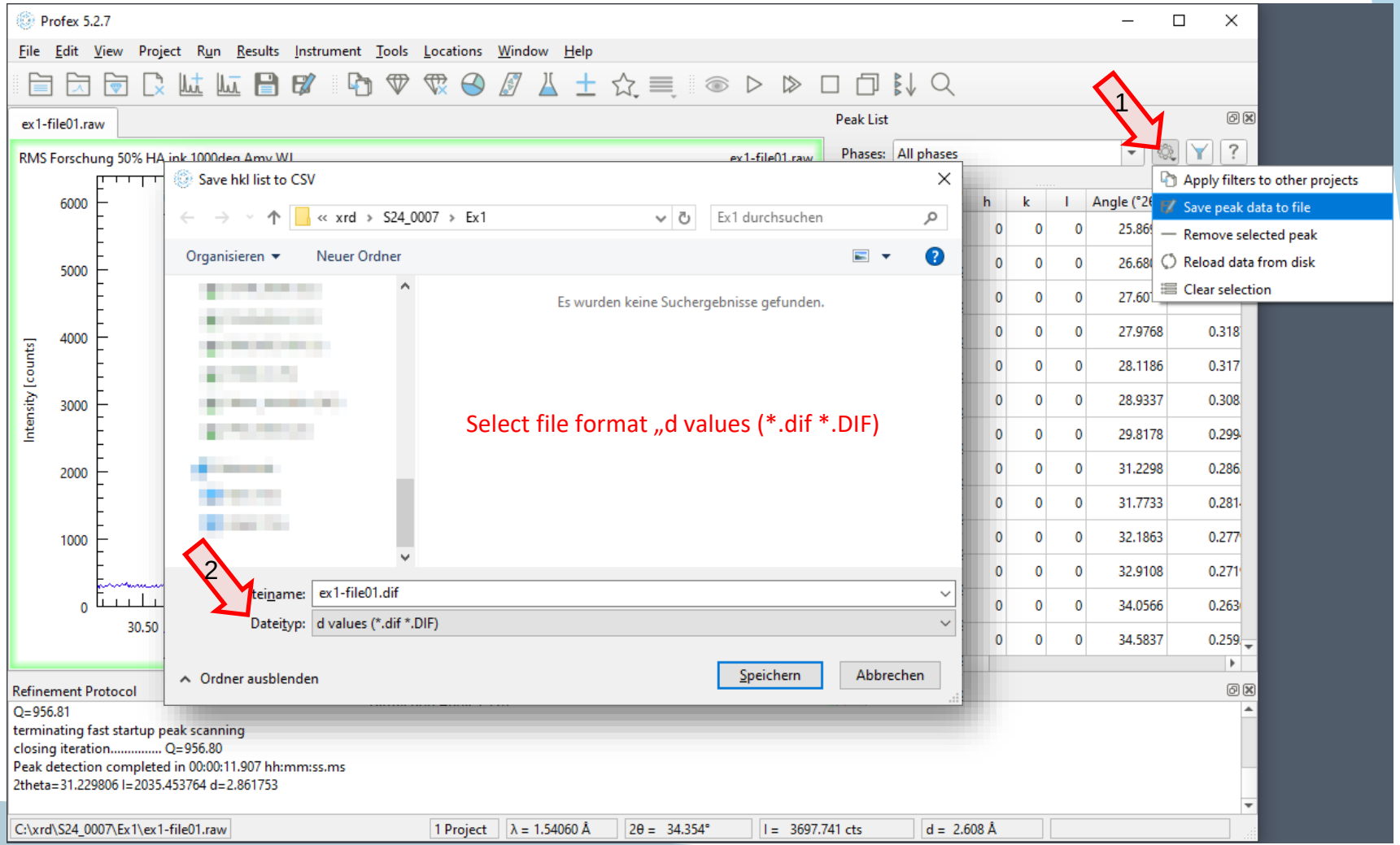


1. Open peak list (Window → Peak List)
2. Run → Peak detection
3. Select instrument and wavelength

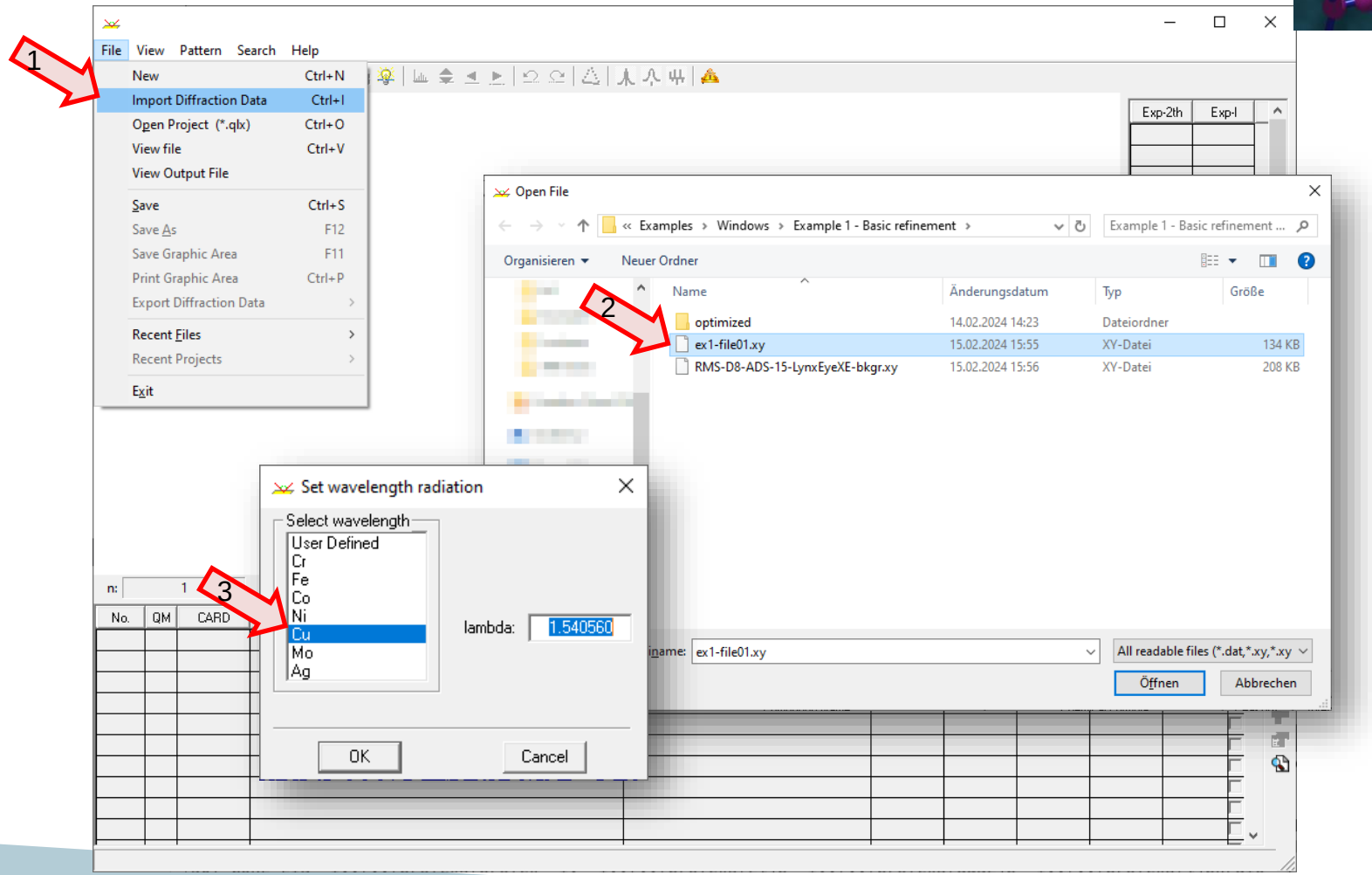
Peak Detection



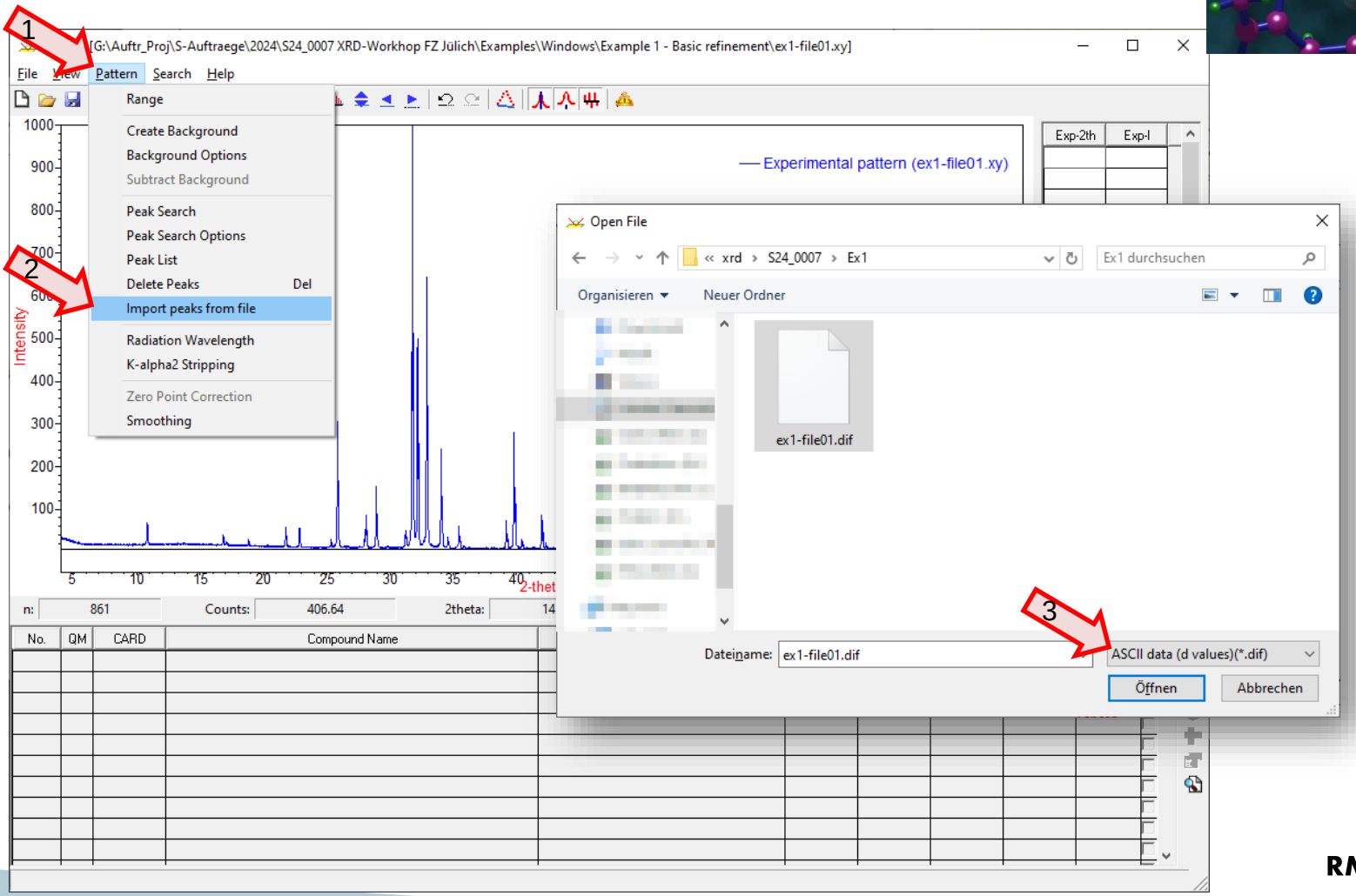
Export Peak List



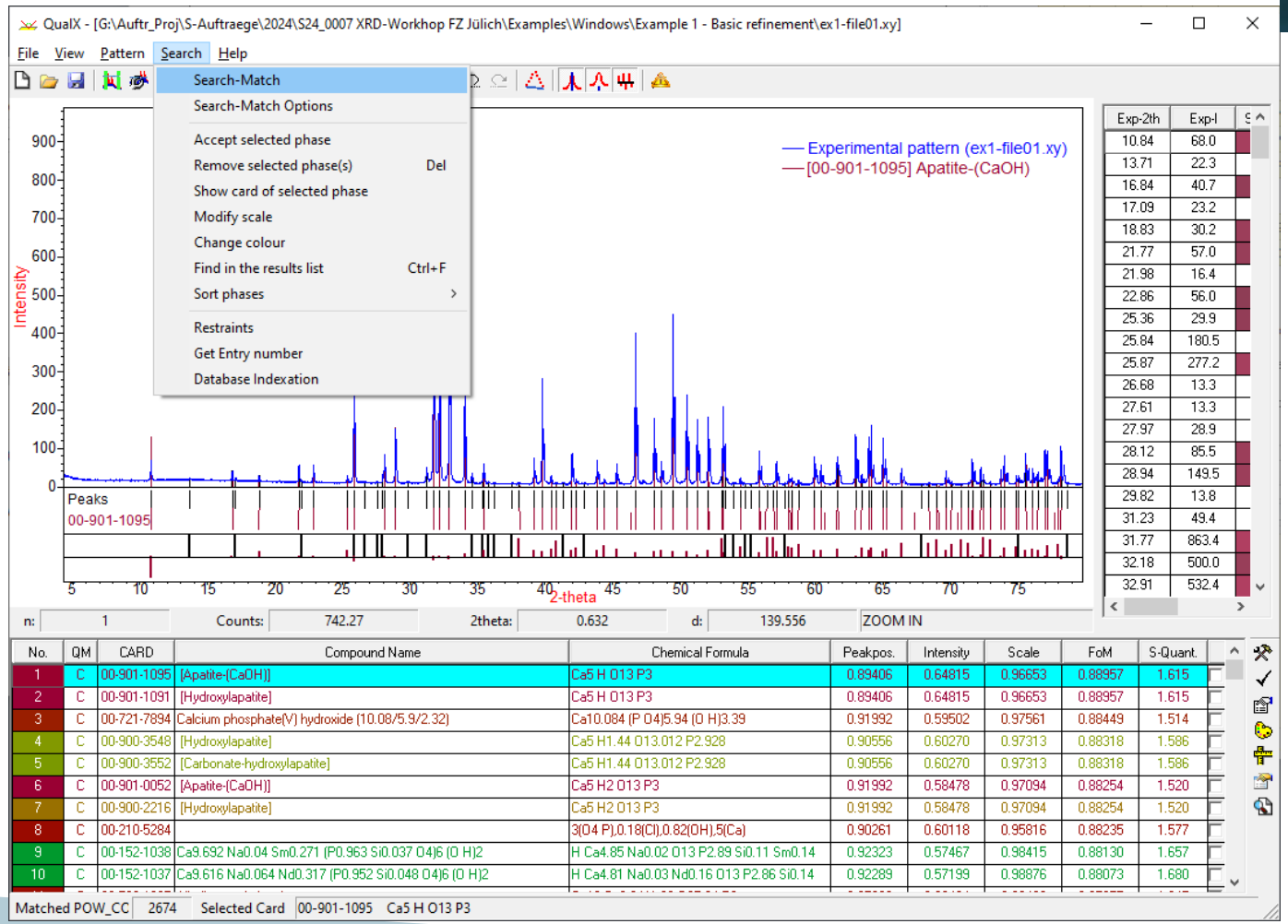
Importing Peak List in QualX2



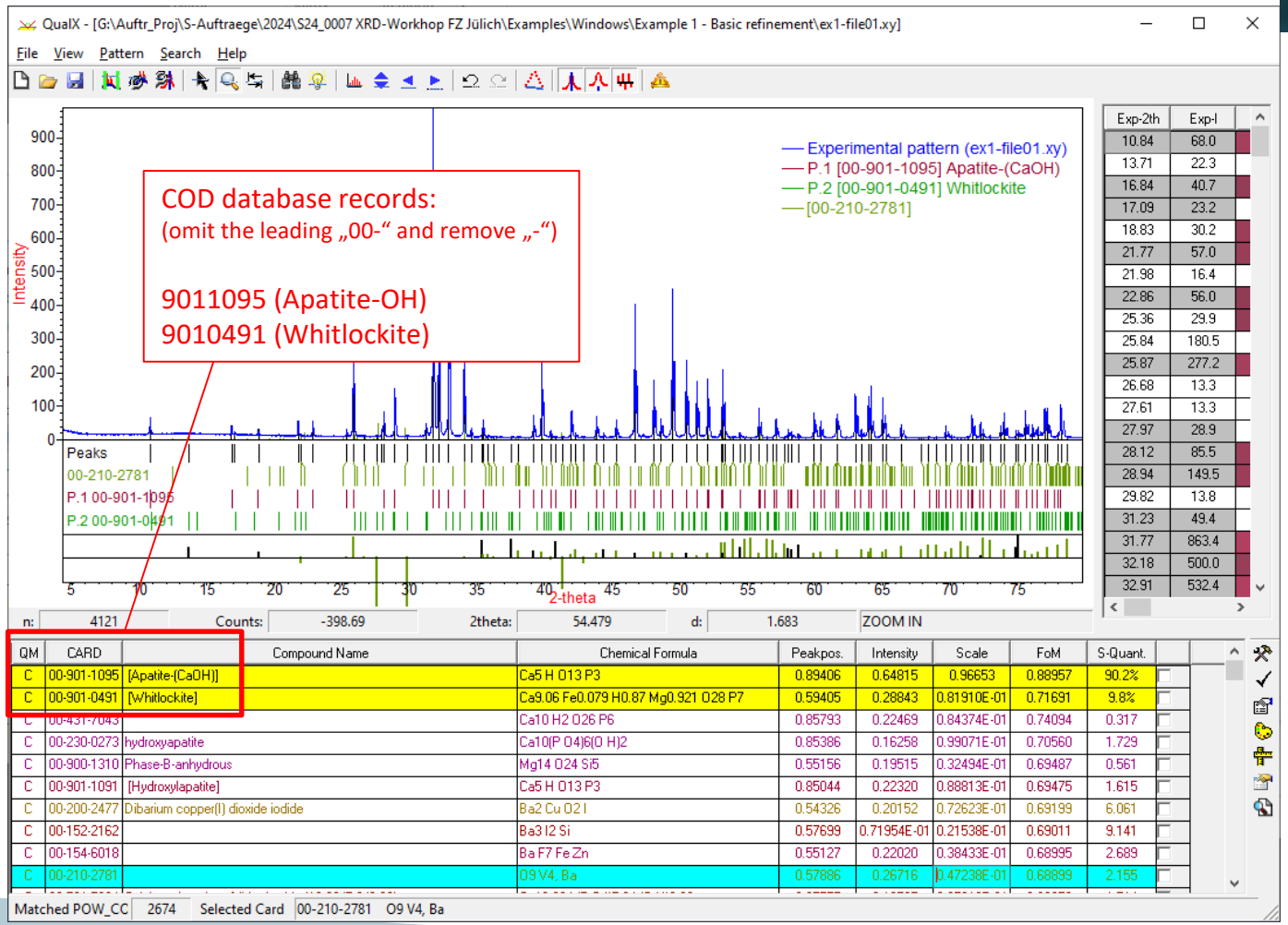
Importing Peak List in QualX2



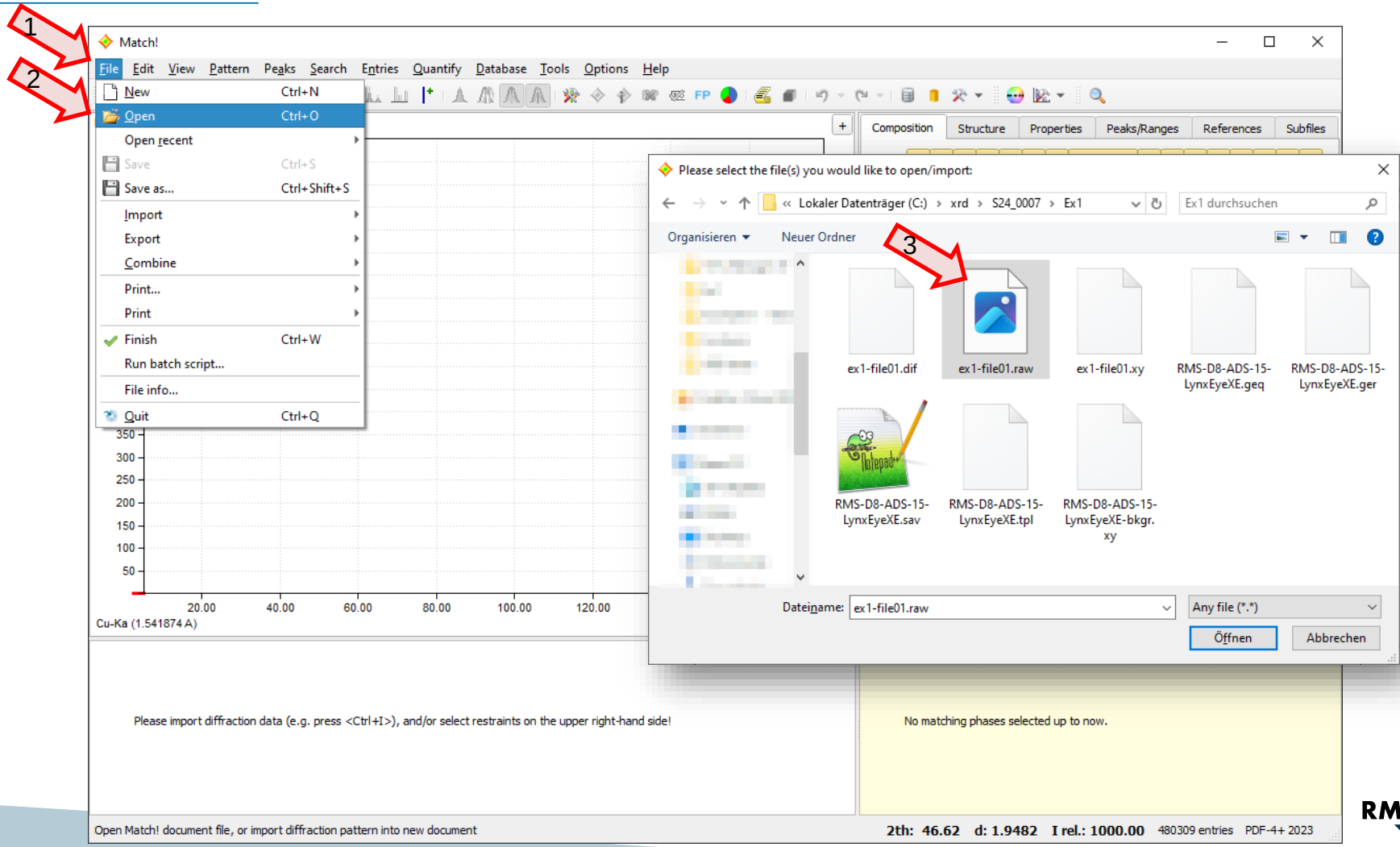
Search/Match in QualX2



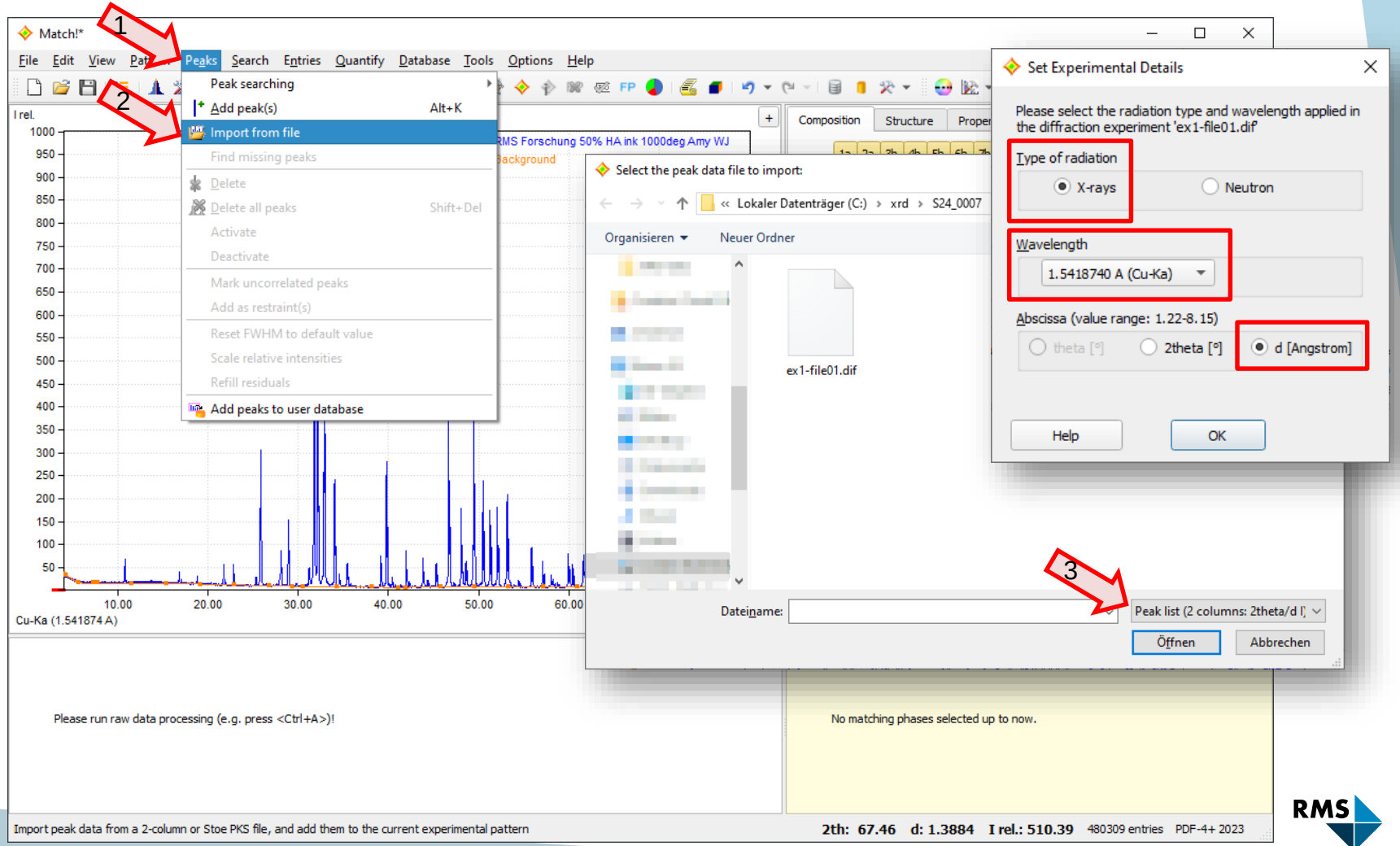
Search/Match in QualX2



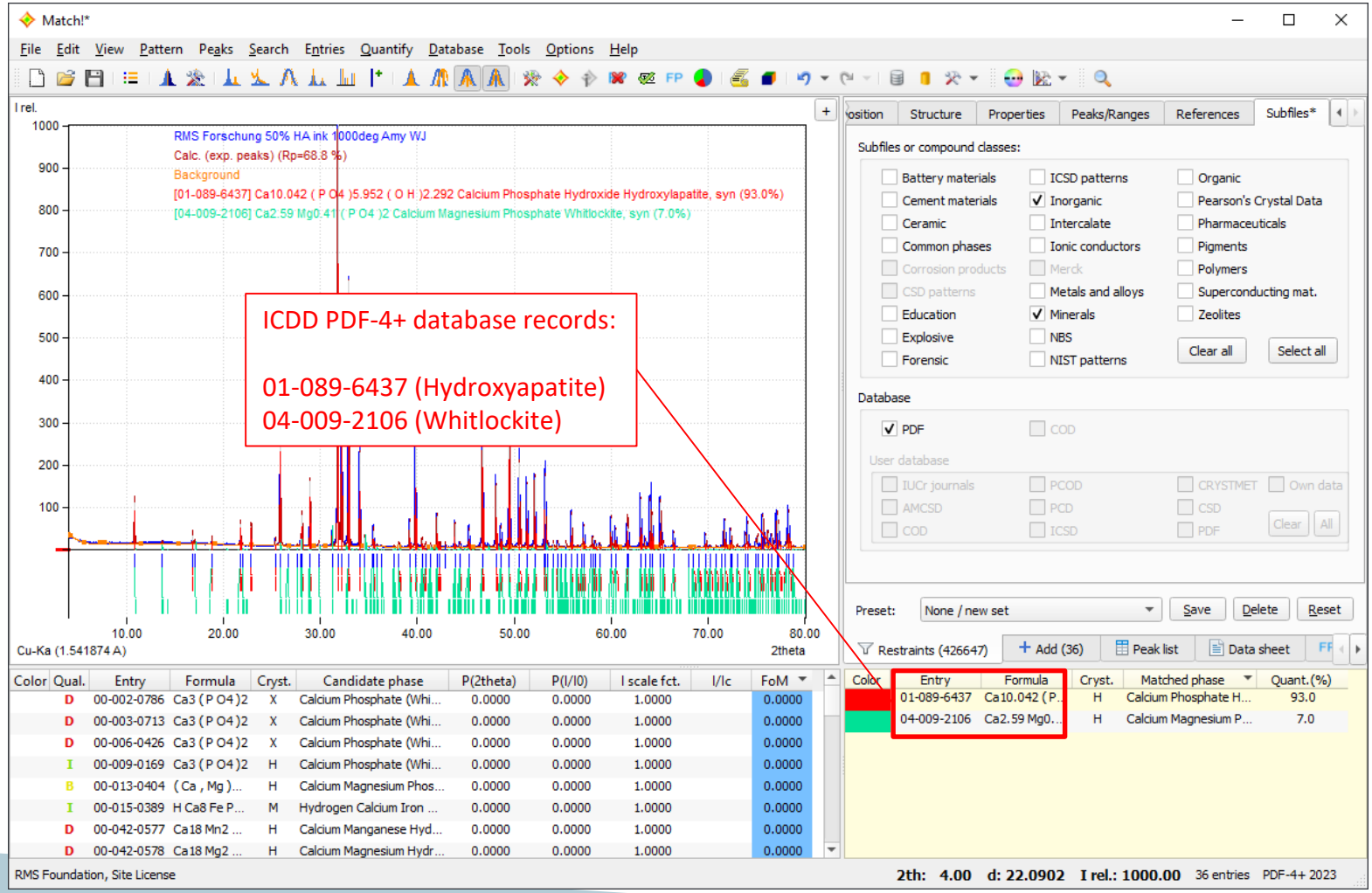
Importing Peak List in Match!



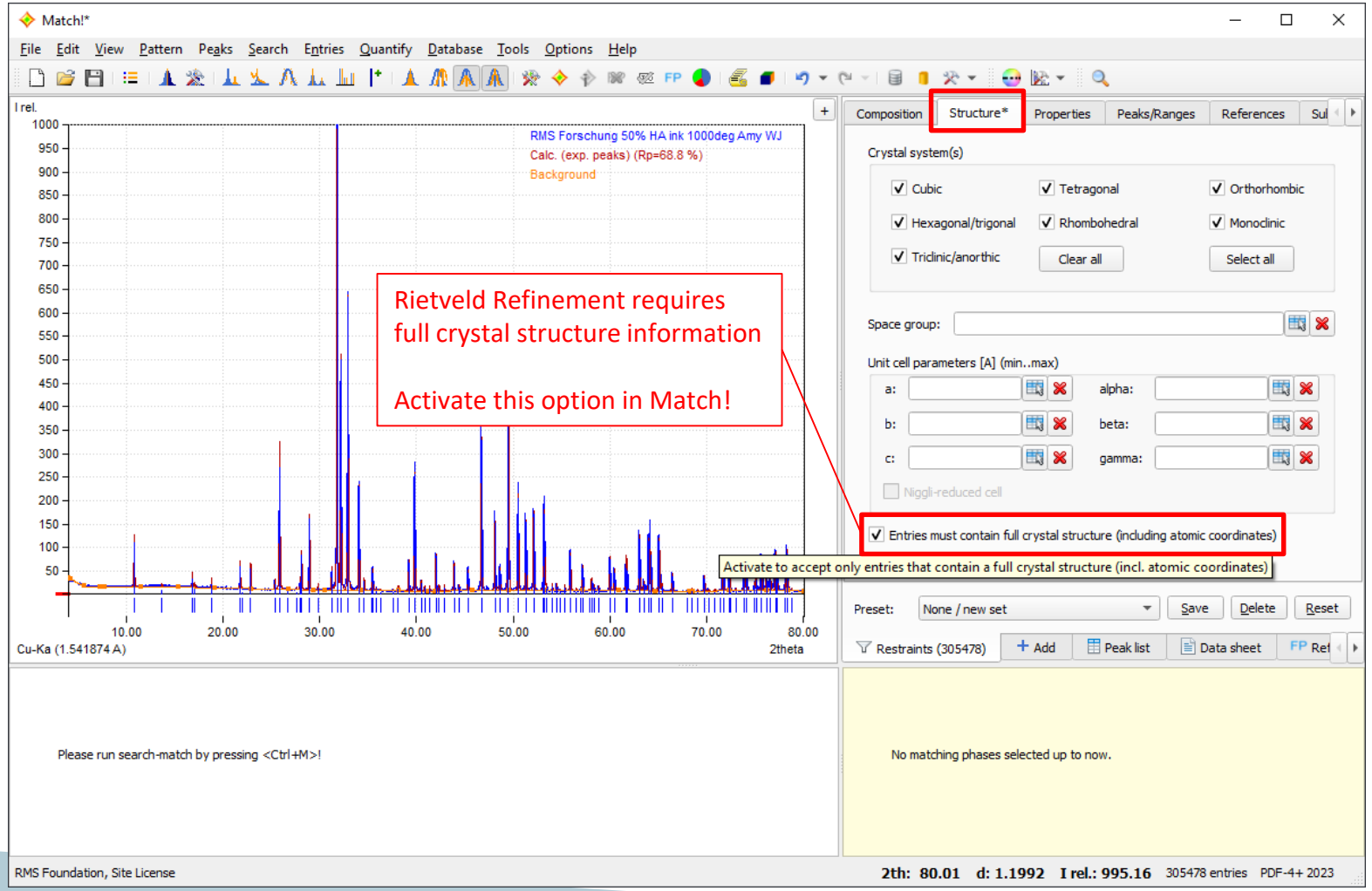
Importing Peak List in Match!



Search/Match in Match!



Matches in Match!



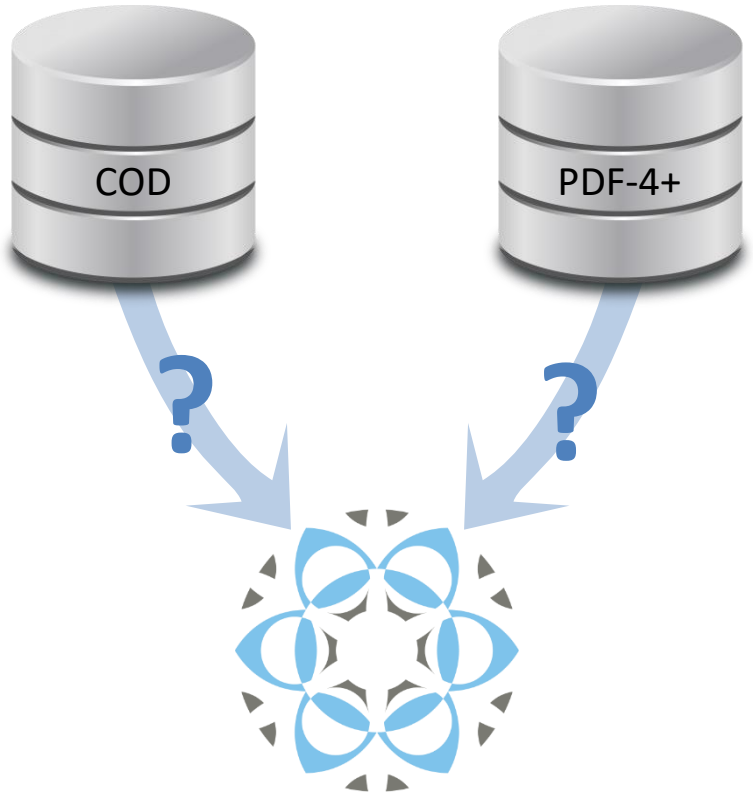
Importing new Structures to Profex

Importing from COD:

- Needs COD installed in Profex
- Needs internet connection

Importing from ICDD PDF-4+

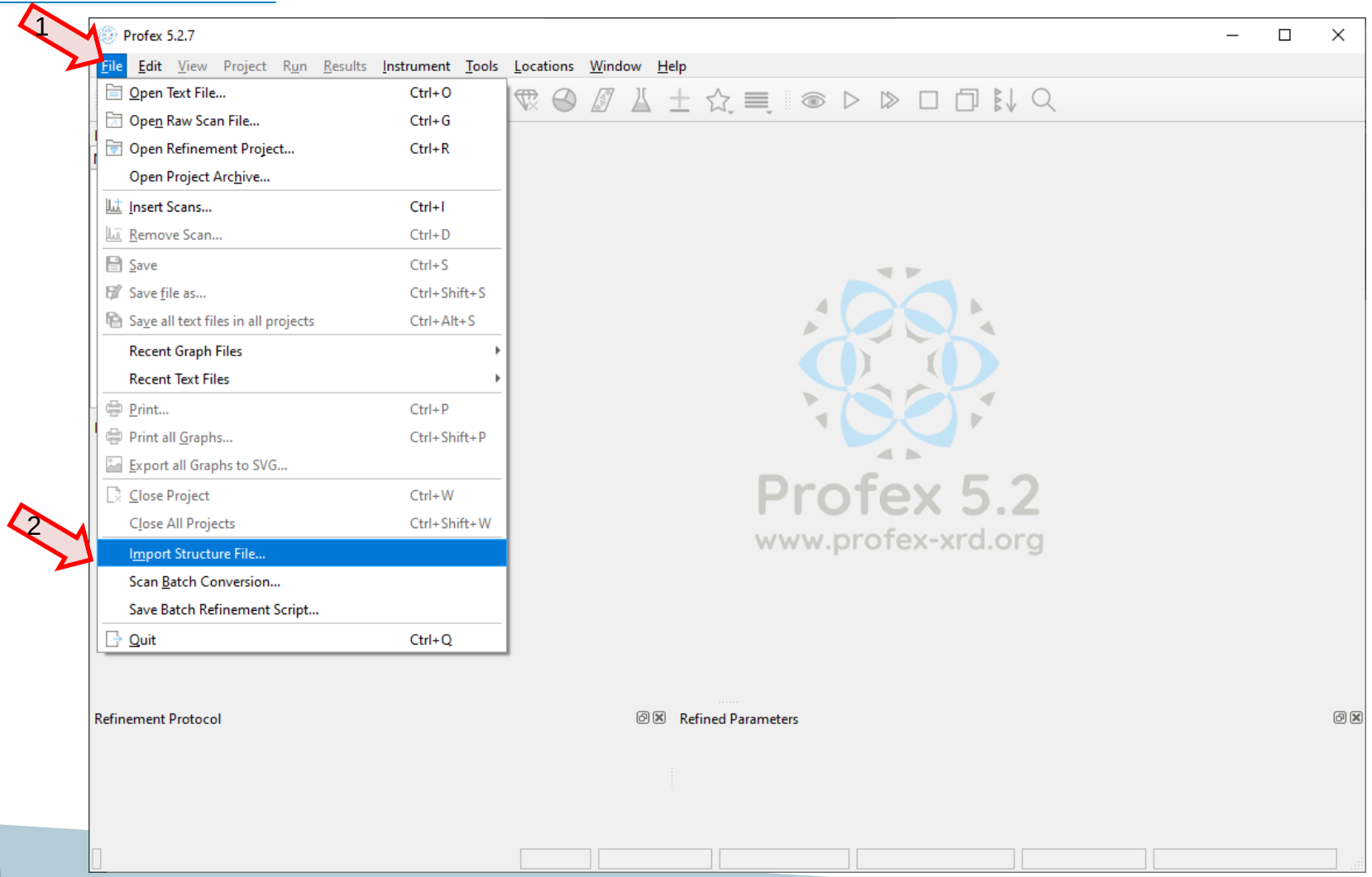
- Needs valid license for PDF-4+
- Export structure from PDF-4+ as XML file



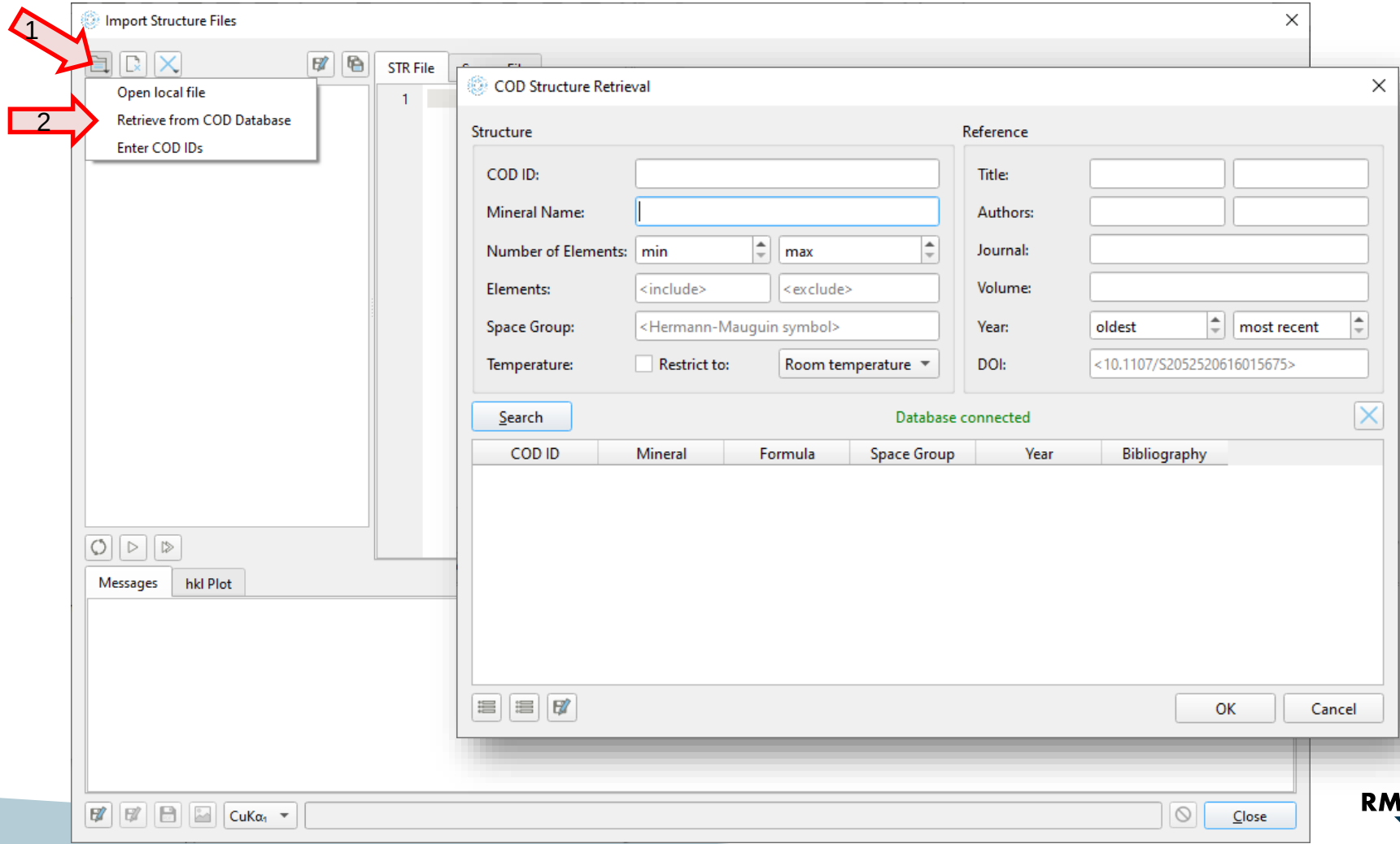
Note:
ICDD **PDF-2** does not contain crystal structure information.

→ Can‘t be used for Rietveld Refinement

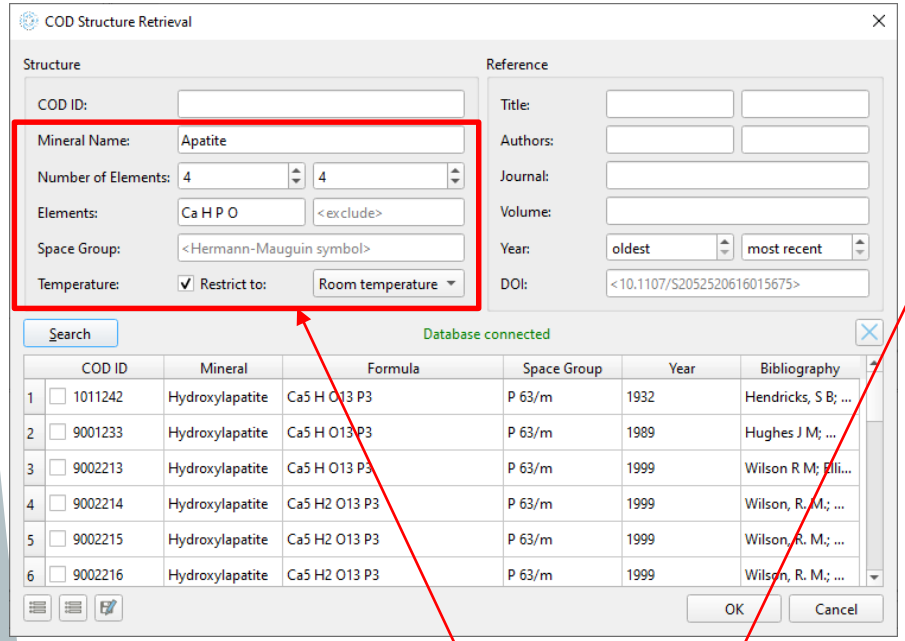
Importing Structure Files from COD

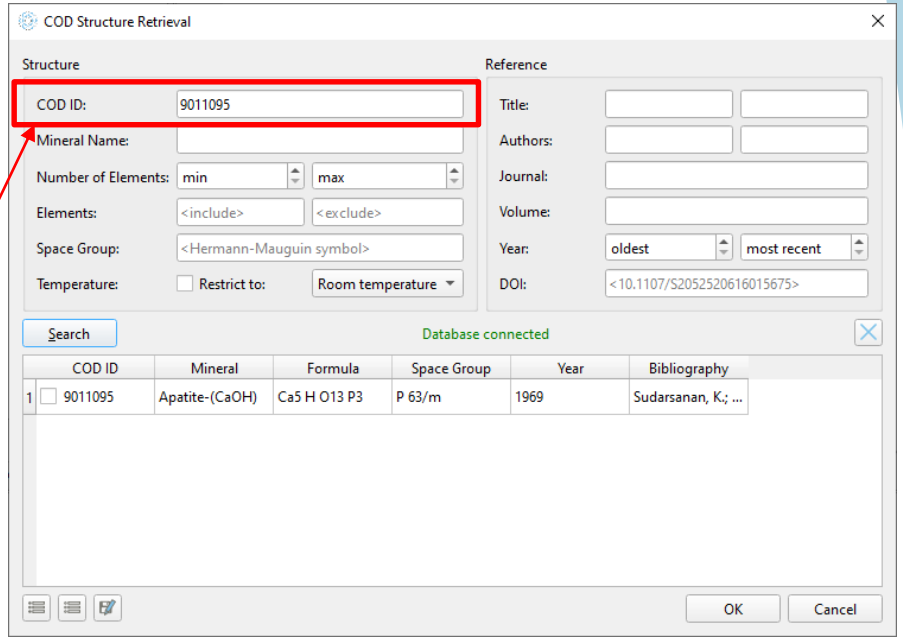


Importing Structure Files from COD

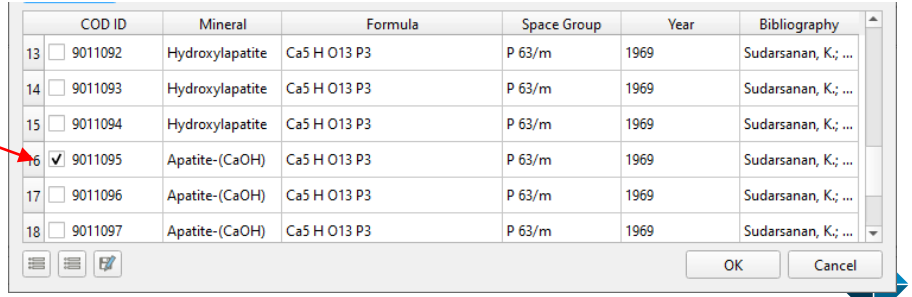


Importing Structure Files from COD

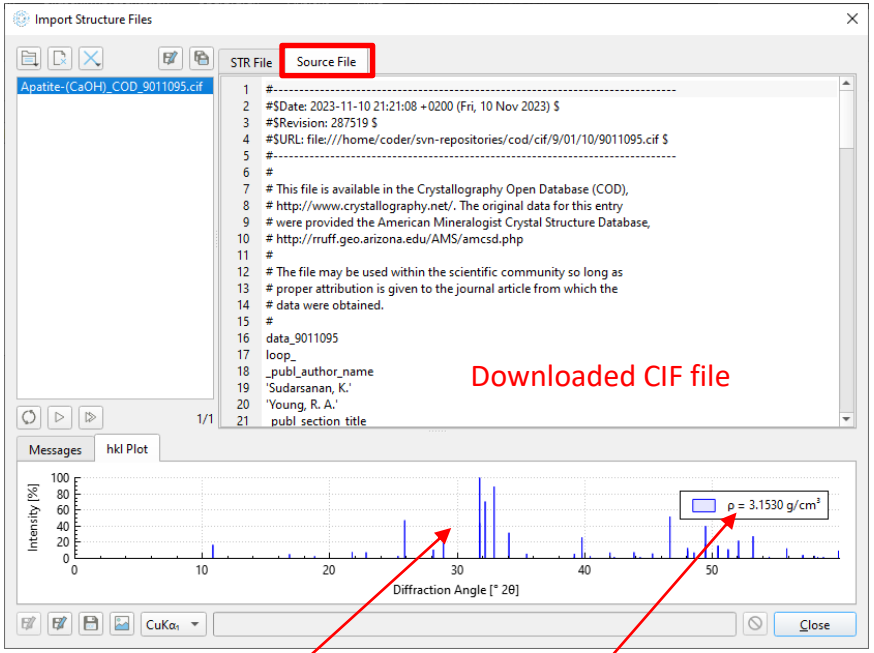


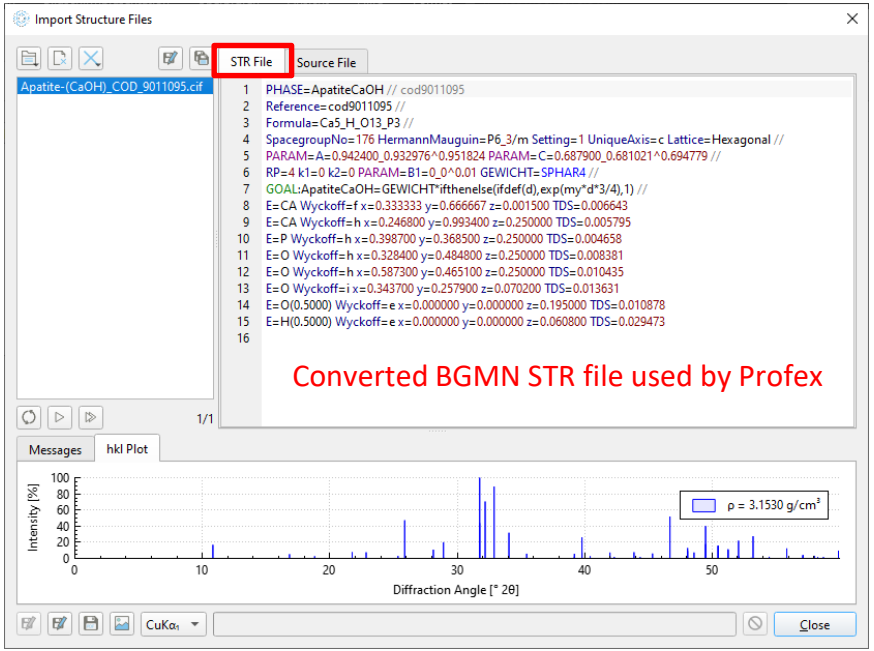


1. Enter mineral properties or COD ID
2. Click «Search»
3. Check the phases you want to download
4. Click «OK» to download

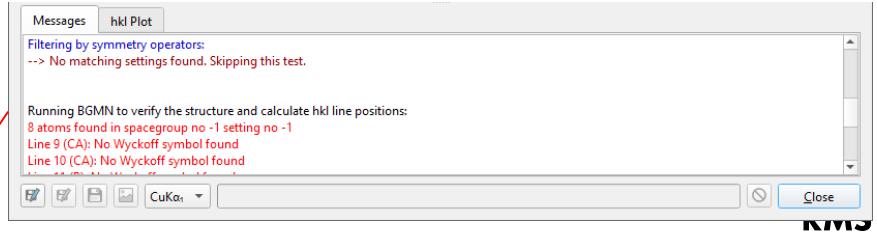


Importing Structure Files from COD



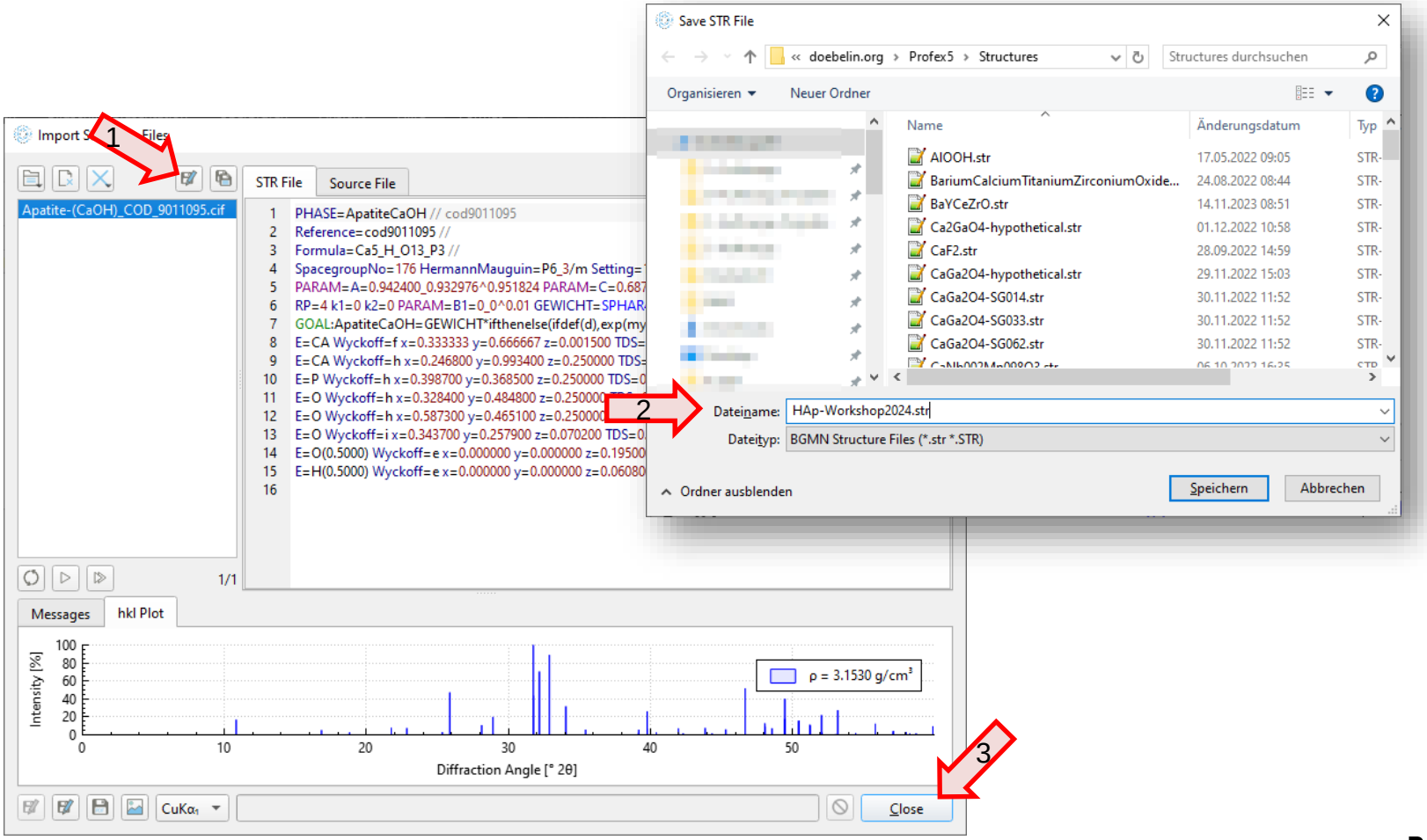


Stick pattern and calculated density for verification

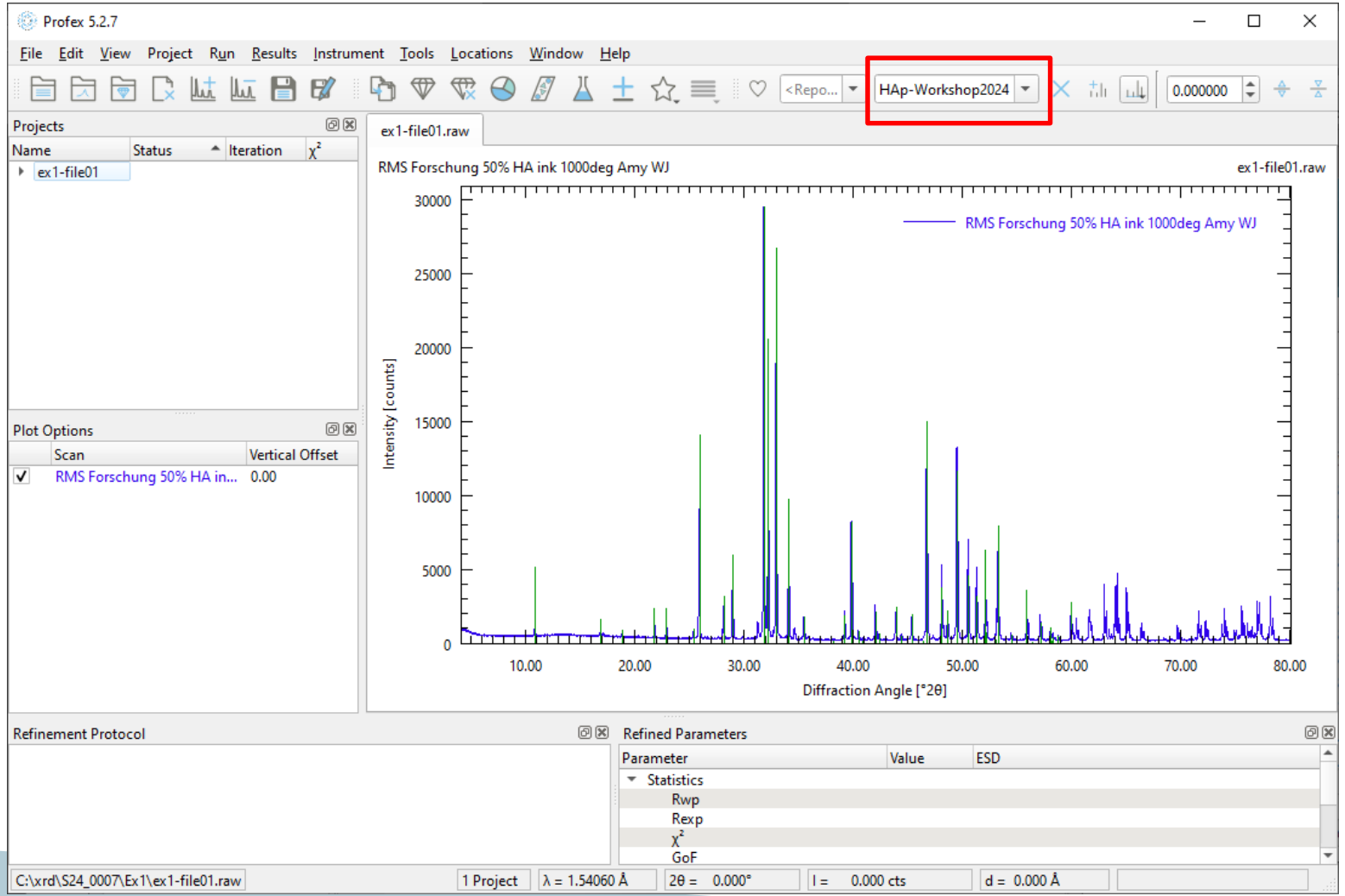


If conversion fails due to corrupted CIF file, no stick pattern is shown and errors are reported in «Messages» protocol.

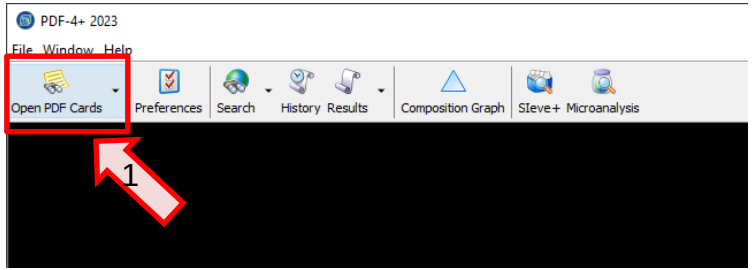
Saving STR Files

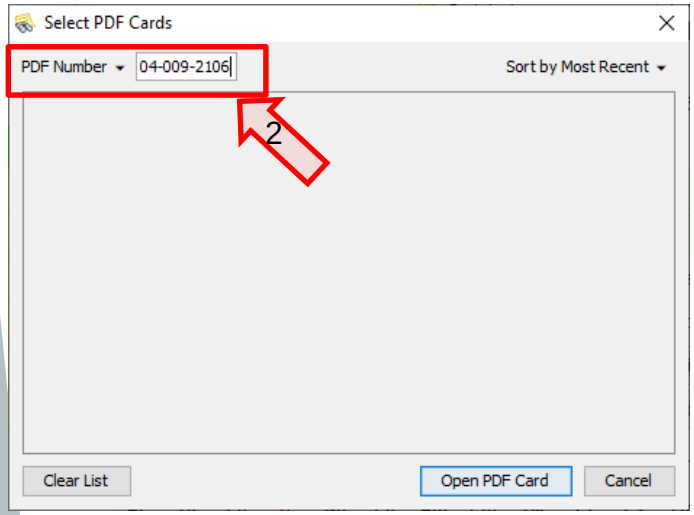


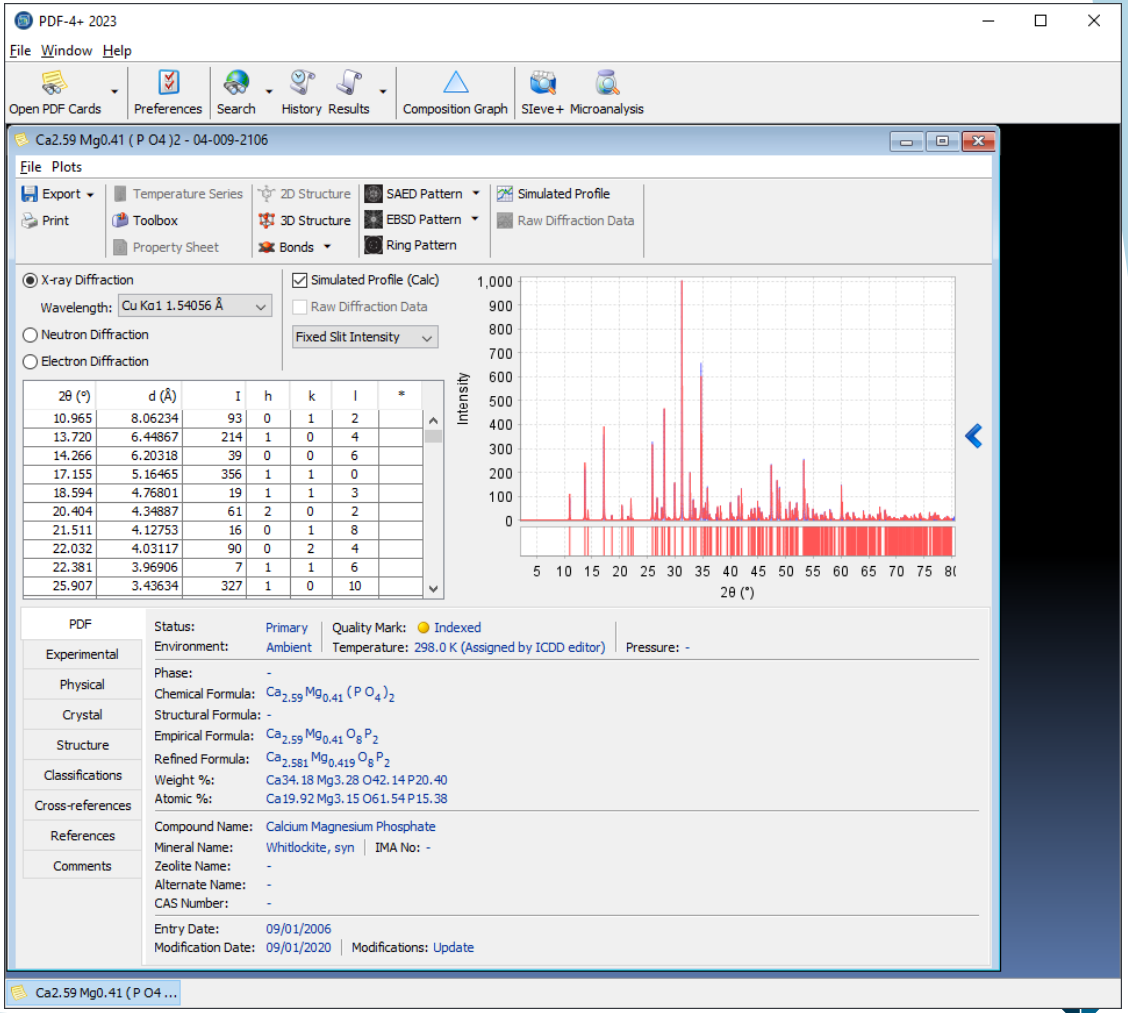
Saving STR Files



Exporting XML from PDF-4+



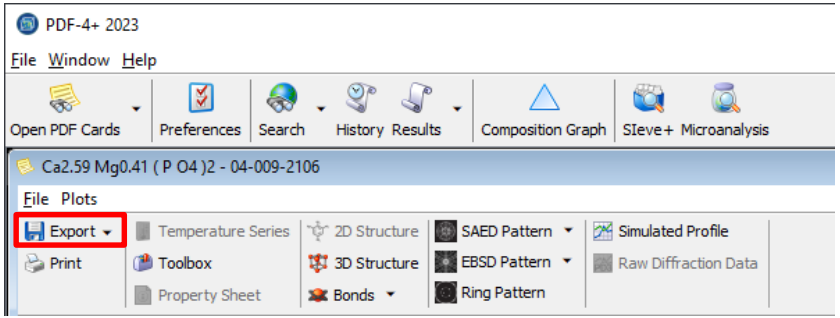


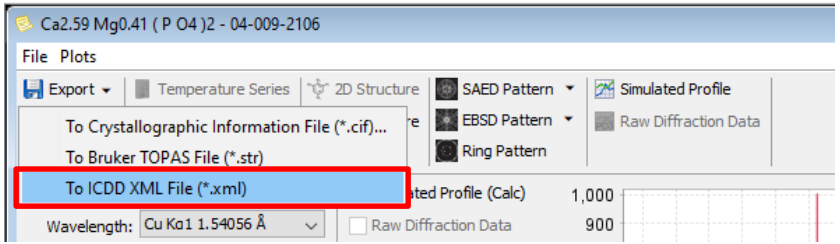


Exporting XML from PDF-4+ / Importing in Profex

In PDF-4+:

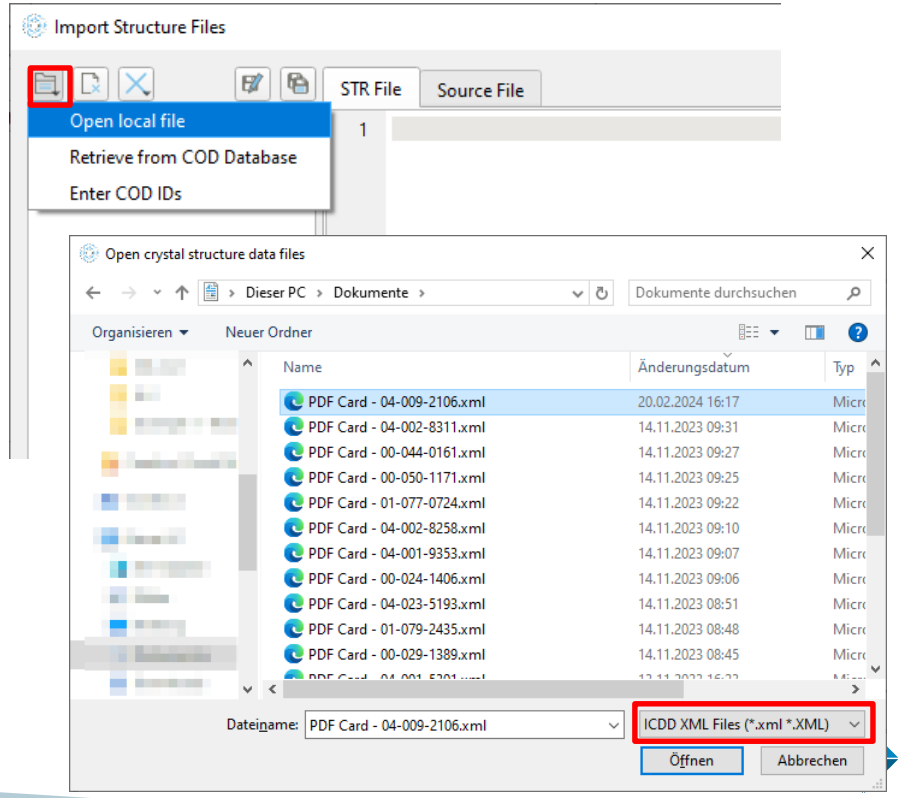
On the PDF card, click Export → To ICDD XML File





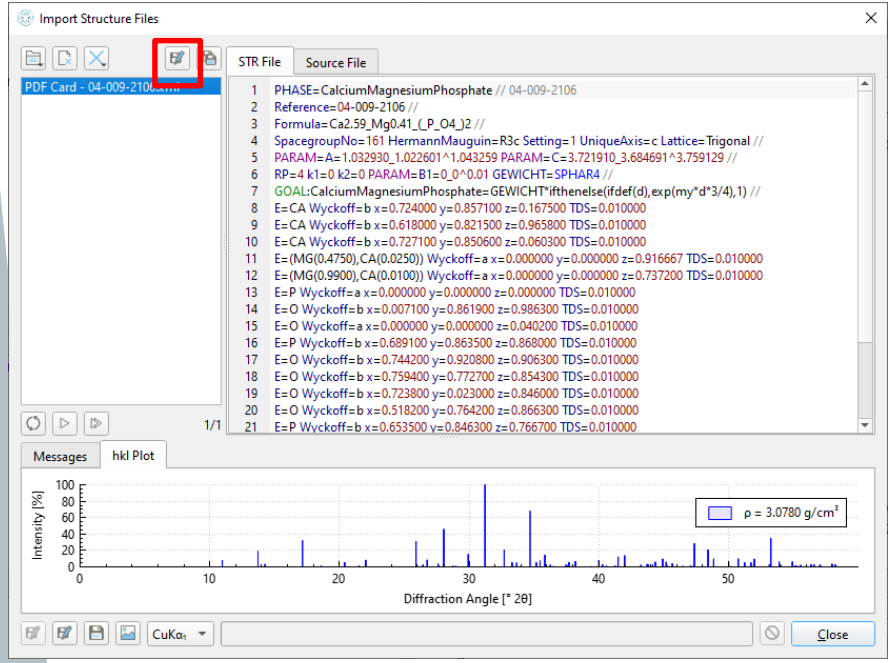
In Profex:

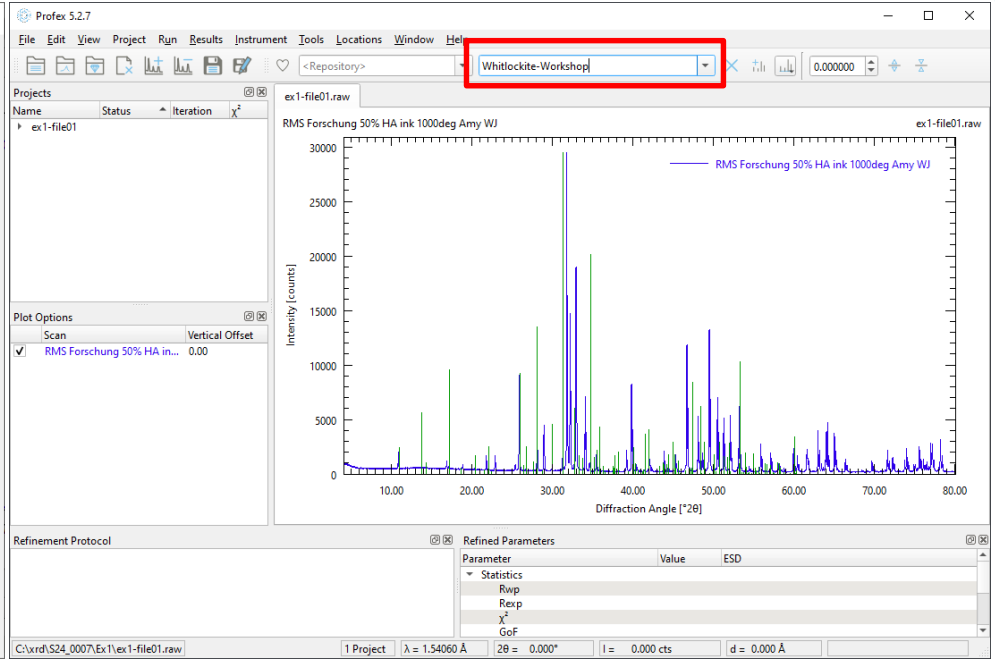
File → Import Structure Files → Open local file
Set file format to „ICDD XML Files“



Saving STR Files

1. Check the stick pattern and density for plausibility
2. Save the STR file
3. Close the import dialog





Phase Identification: Summary

- All phases identified
  - double-click
  - search-match module
  - 3rd party software
- Missing structure files retrieved from COD or PDF-4+ (or other source)
- Retrieved structure files converted from CIF/XML format to STR
- Next: Rietveld refinement