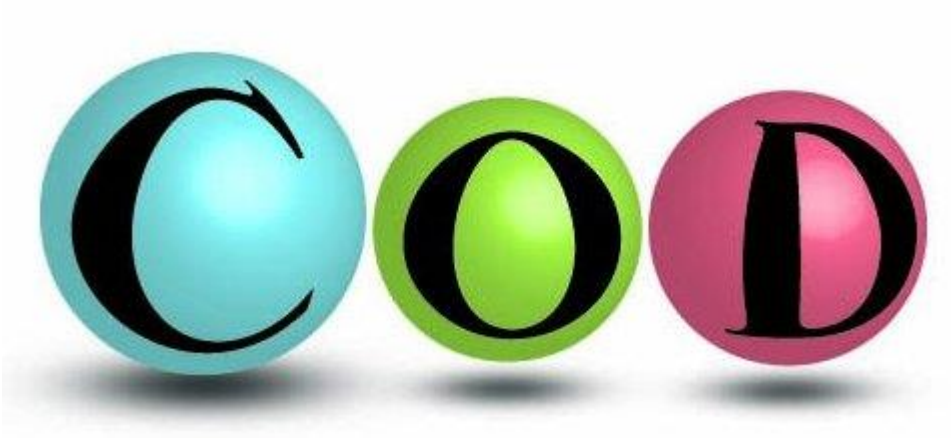
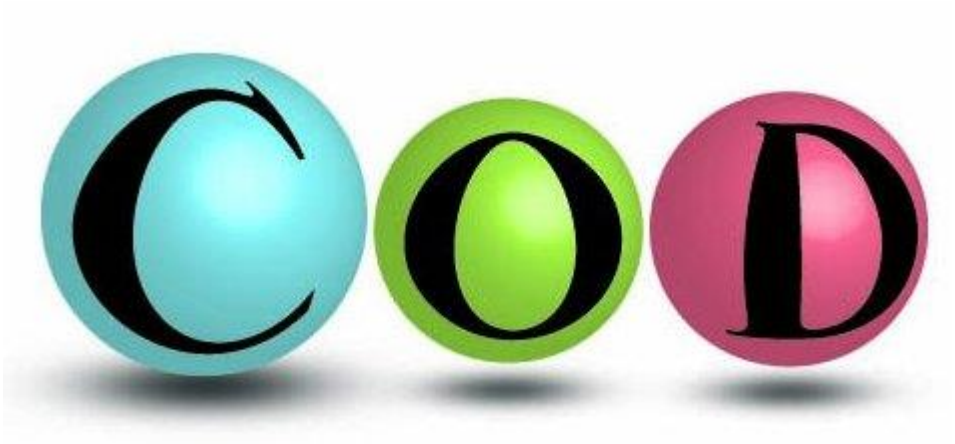
RÉCIPROCS
conditions extrêmes

Un petit tour de la



Crystallography Open Database

avec Benoît Baptiste et Olivier Pérez

La 

… et son environnement

https://www.iucr.org/resources/data https://www.afc.asso.fr/documentation/bases-de-donnees

Crystallography databases : money

The Cambridge Crystallographic Data Centre

https://www.ccdc.cam.ac.uk/ (1965)

Organic and metal-organic compounds
900000 entries

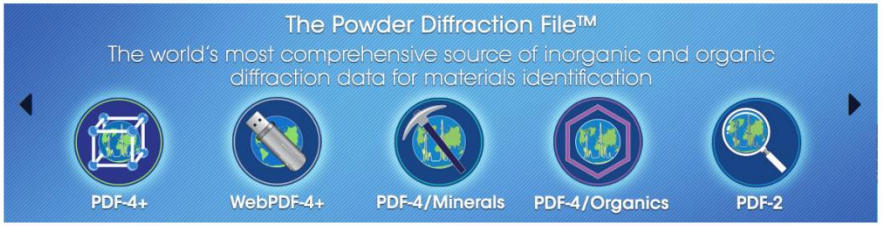
FIZ Karlsruhe ICSD

http://www2.fiz-karlsruhe.de/icsd_home.html (1978)

Inorganic compounds - 190000 entries

ICDD®
INTERNATIONAL CENTRE FOR DIFFRACTION DATA

http://www.icdd.com/ (1941)



Materials science (890000 diffraction patterns and 330000 crystal structures)
X-ray, electron and neutron diffraction
Modulated structures (since 2011)
Amorphous, poorly crystalline, nanomaterials disordered clays and polymers
11300 raw diffraction patterns

https://www.iucr.org/resources/data https://www.afc.asso.fr/documentation/bases-de-donnees

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The Cambridge Crystallographic

http 1965)

Organic mpounds

https://bib.cnrs.fr/

FIZ Karlsruhe ICSD

http://www2.fiz tml (1978)

Inorganic c ntries

https://bib.cnrs.fr/

but INC only !

ICDD®
INTERNATIONAL CENTRE FOR DIFFRACTION DATA

http://www.icdd.com/ (1941)

The Powder Diffraction File™
The world's most comprehensive source of inorganic and organic diffraction data for materials identification

PDF-4+ WebPDF-4+ PDF-4/Minerals PDF-4/Organics PDF-2

Materials science (890000 diffraction patterns and 330000 cry
X-ray, electron and neutron diffraction
Modulated structures (since 2011)
Amorphous, poorly crystalline, nanomaterials disordered c
11300 raw diffraction patterns

https://bib.cnrs.fr/

soon ?

https://www.iucr.org/resources/data https://www.afc.asso.fr/documentation/bases-de-donnees

Crystallography databases : open access

RCSB PDB
PROTEIN DATA BANK

44188 Distinct Protein Sequences | **38551** Structures of Human Sequences | **10044** Nucleic Acid Containing Structures

https://www.rcsb.org/ (1971)

ndb NUCLEIC ACID DATABASE

http://ndbserver.rutgers.edu/ (1992)

Biological macromolecules

X-ray, NMR & electron - 120000 entries

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UA Mineralogy | Caltech Mineralogy

RRUFF

http://rruff.info/ - IR, Raman, XRD - 4000 records

Mineralogy Database

http://webmineral.com/ - 4700 entries

http://database.iem.ac.ru/mincryst/ (1997) 9800 records

American Mineralogist Crystal Structure Database

http://rruff.geo.arizona.edu/AMS/amcsd.php (2000)
4000 records

Minerals

https://www.iucr.org/resources/data https://www.afc.asso.fr/documentation/bases-de-donnees

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4000 records

Minerals

COD

http://www.crystallography.net/cod/ (2003)

Organic, metal-organic, inorganic, minerals

X-ray, electron & neutron - 376000 records

TCOD

mpod

https://www.iucr.org/resources/data https://www.afc.asso.fr/documentation/bases-de-donnees

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Mineralogy Database

http://webmineral.com/ - 4700 entries

WWW-MINCRYST

Crystallographic and Crystallochemical Database for Minerals and their Structural Analogues

Кристаллографическая и кристаллохимическая База данных для минералов и их структурных аналогов

English Russian

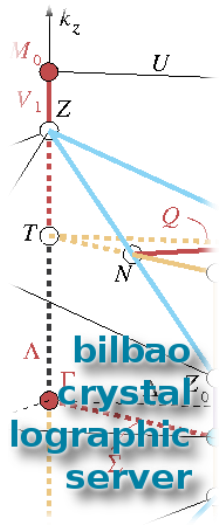
http://database.iem.ac.ru/mincryst/ (1997) 9800 records

American Mineralogist Crystal Structure Database

http://rruff.geo.arizona.edu/AMS/amcsd.php (2000)

4000 records

Minerals



Magnetic, incommensurate and modulated structures

148 entries

COD

http://www.crystallography.net/cod/ (2003)

Organic, metal-organic, inorganic, minerals

X-ray, electron & neutron - 376000 records

bilbao crystallographic server

http://www.cryst.ehu.es/ (1997)

Properties of crystallographic symmetry groups

TCOD

mpod

https://www.iucr.org/resources/data https://www.afc.asso.fr/documentation/bases-de-donnees

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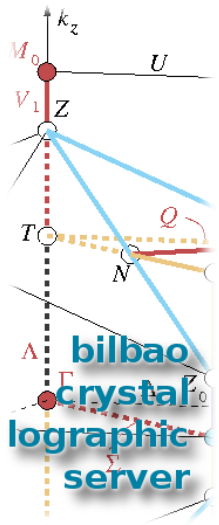

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http://www.cryst.ehu.es/ (1997)

Properties of crystallographic symmetry groups

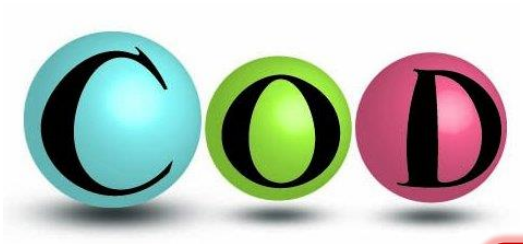
TCOD

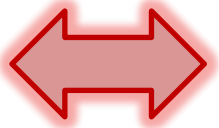
mpod

Database of Zeolite Structures

http://www.iza-structure.org/databases/

Interoperations between databases :

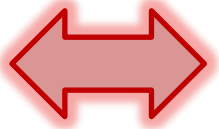




American Mineralogist Crystal Structure Database

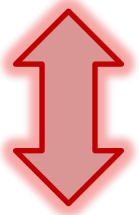
To use features of software environment

RCSB PDB PROTEIN DATA BANK



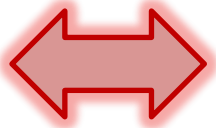
ndb NUCLEIC ACID DATABASE

To improve the description of ligands for macromolecules



To propose shared services in all chemistry domains

The Cambridge Crystallographic Data Centre



FIZ Karlsruhe ICSD

Some examples …

Open database : Mineralogy Database example

Minerals Arranged by X-Ray Powder Diffraction

See Help on X-Ray Diffraction.

Powder X-ray Diffraction (XRD) is one of the primary techniques used by mineralogists and solid state chemists to examine the physico-chemical make-up of unknown materials. This data is represented in a collection of single-phase X-ray powder diffraction patterns for the three most intense D values in the form of tables of interplanar spacings (D), relative intensities (I/Io), mineral name and chemical formulae

The XRD technique takes a sample of the material and places a powdered sample in a holder, then the sample is illuminated with x-rays of a fixed wave-length and the intensity of the reflected radiation is recorded using a goniometer. This data is then analyzed for the reflection angle to calculate the inter-atomic spacing (D value in Angstrom units - 10^{-8} cm). The intensity(I) is measured to discriminate (using I ratios) the various D spacings and the results are compared to this table to identify possible matches. Note: 2 theta (Θ) angle calculated from the Bragg Equation, 2 Θ = 2(arcsin(n λ/(2d)) where n=1;

For more information about this technique, see X-Ray Analysis of a Solid or take an internet course at Birkbeck College On-line Courses. Many thanks to Frederic Biret for these data.

Optional Search Query - To Reset, Click Here

Selected X-Ray λ	Change X-Ray λ	D_1 Å	D_2 Å	D_3 Å	Tolerance %	Elements	
1.54056 - CuKa1		3.34			10	SiO2	Valider

[1]

Listing of 6 Records Sorted by D_1 using 1.54056 - CuKa1 for 2θ WHERE (d1 > 3.006 AND d1 < 3.674) AND (formula LIKE 'SiO2')

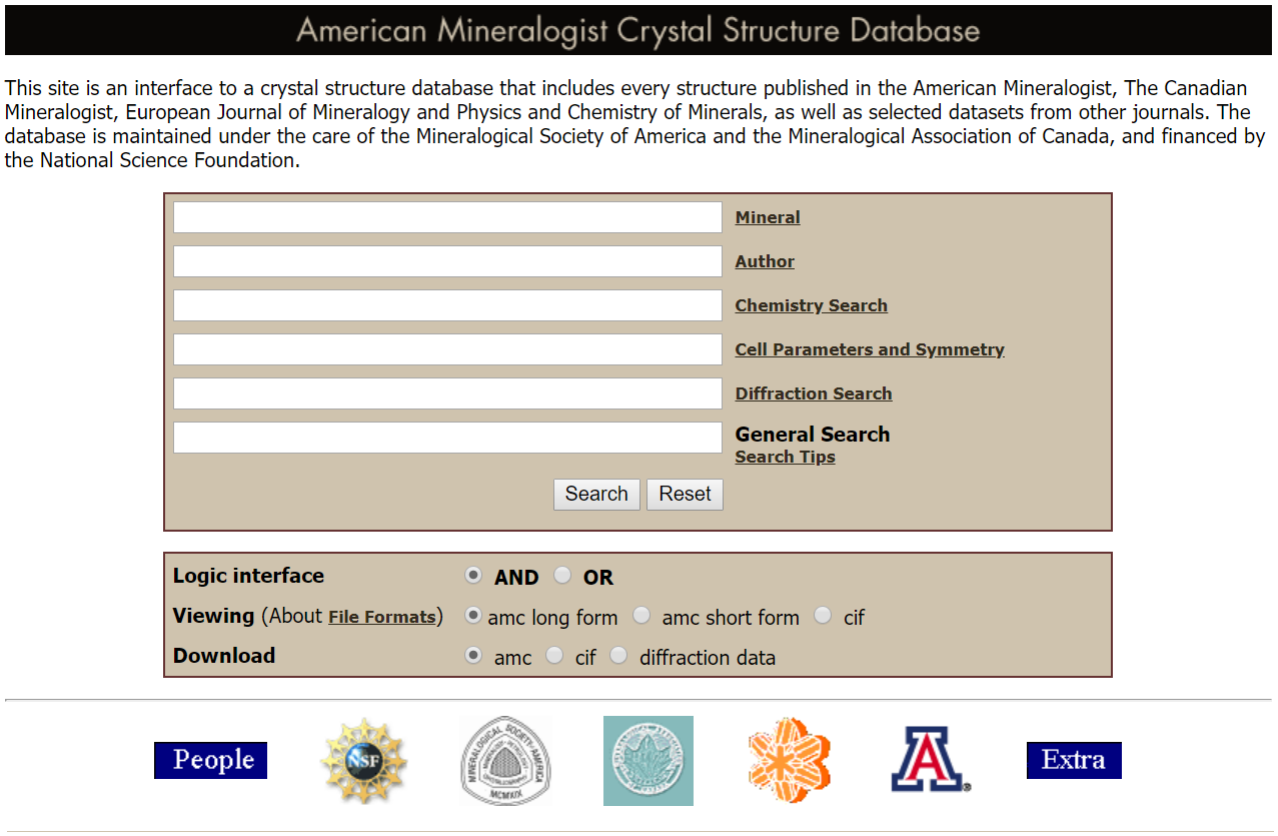
D_1 Å (2θ)	I_1 %)	D_2 Å (2θ)	I_2 (%)	D_3 Å (2θ)	I_3 (%)	Mineral	Formula
3.098(28.79)	100	3.432(25.94)	50	2.770(32.29)	15	Coesite	SiO2
3.335(26.71)	100	4.430(20.03)	90	3.391(26.26)	58	Moganite	SiO2
3.342(26.65)	100	4.257(20.85)	22	1.818(50.14)	14	Quartz	SiO2
3.390(26.27)	50	1.370(68.42)	100	1.380(67.86)	100	Lutecite	SiO2
3.390(26.27)	50	1.380(67.86)	100	1.370(68.42)	100	Lutecite	SiO2
3.390(26.27)	50	1.380(67.86)	100	1.830(49.79)	100	Lutecite	SiO2

[1]

a quick search with 3 peaks

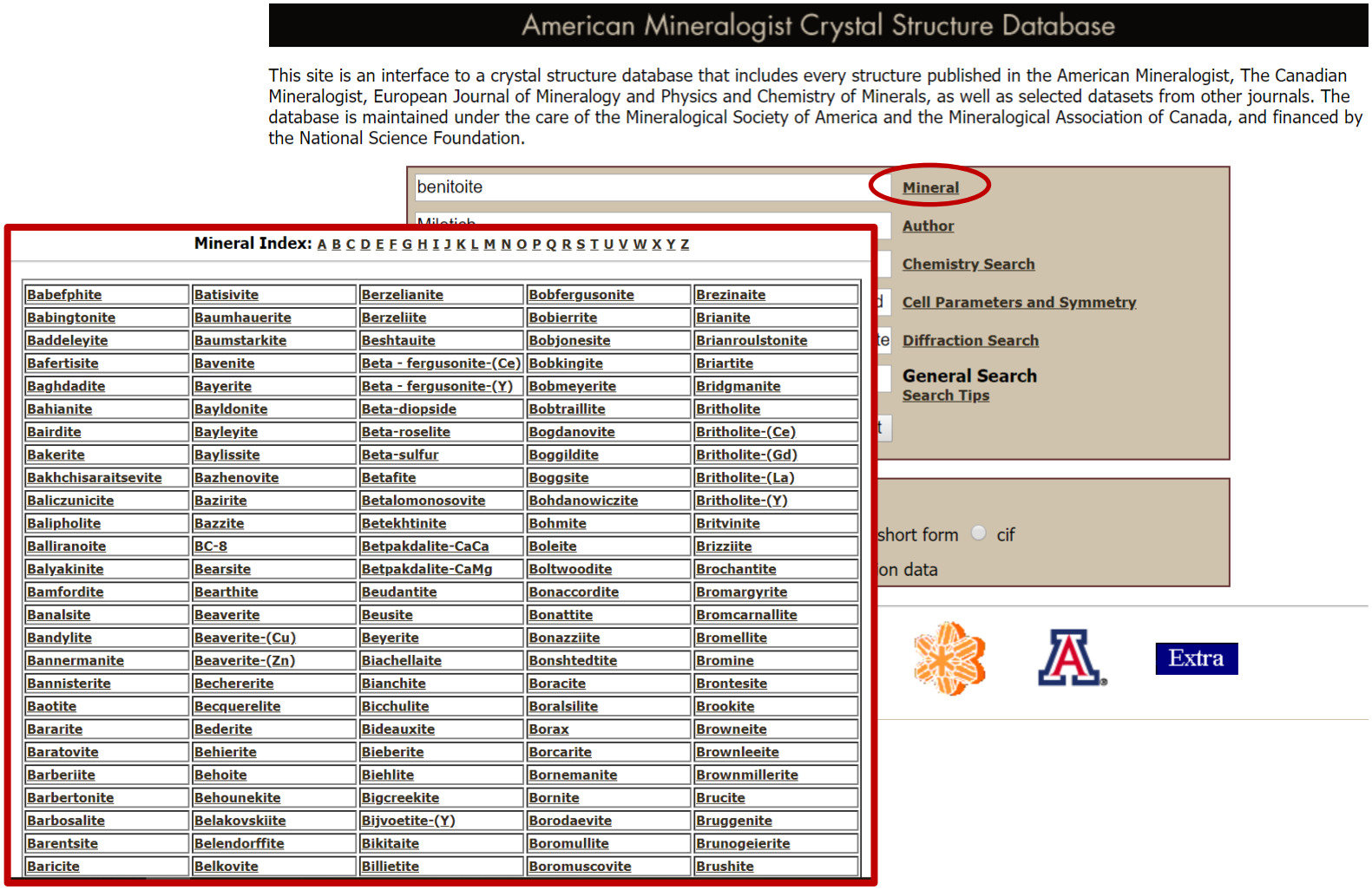
http://webmineral.com/

Open database : AMCSD example



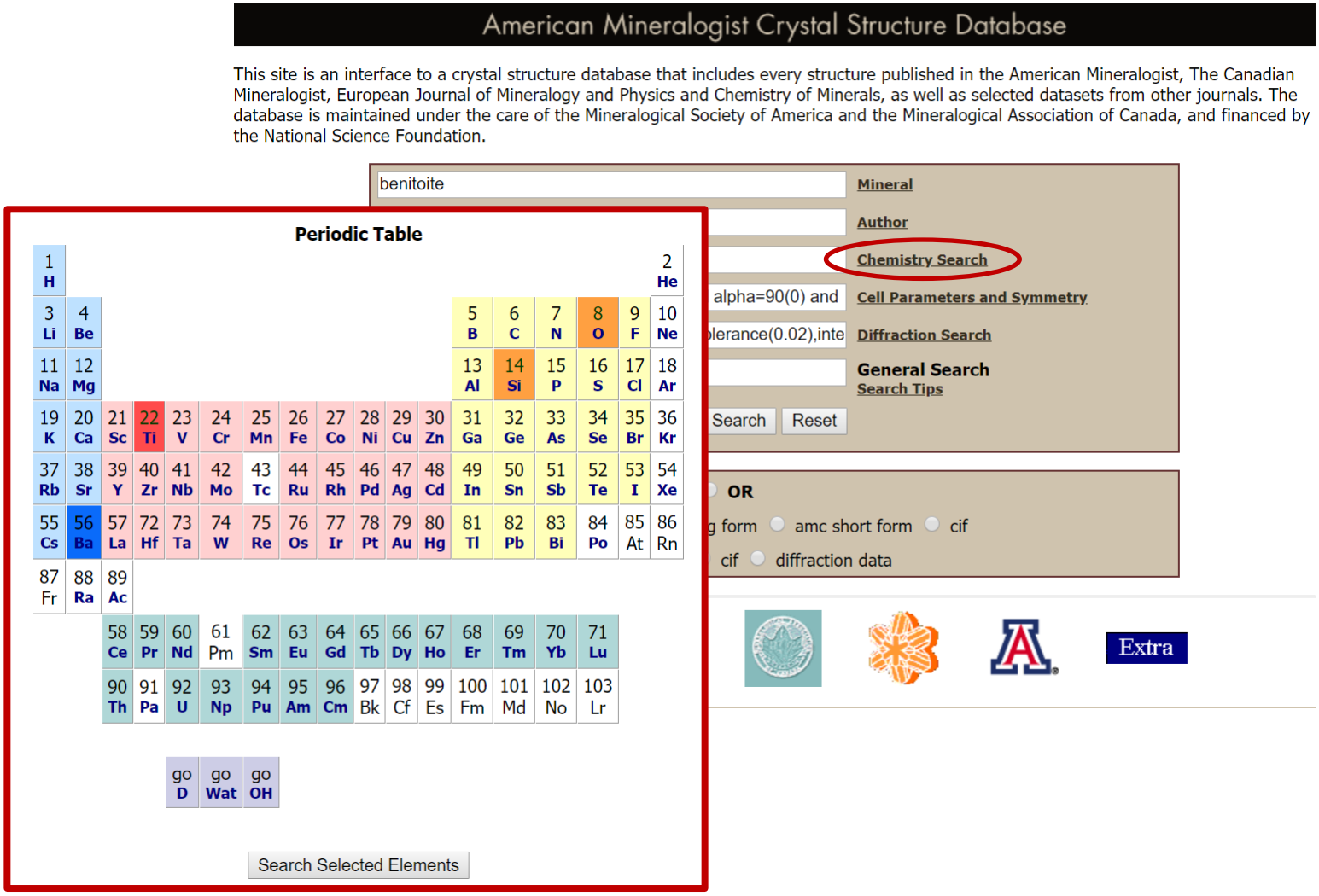
http://rruff.geo.arizona.edu/AMS/amcsd.php

Open database : AMCSD example



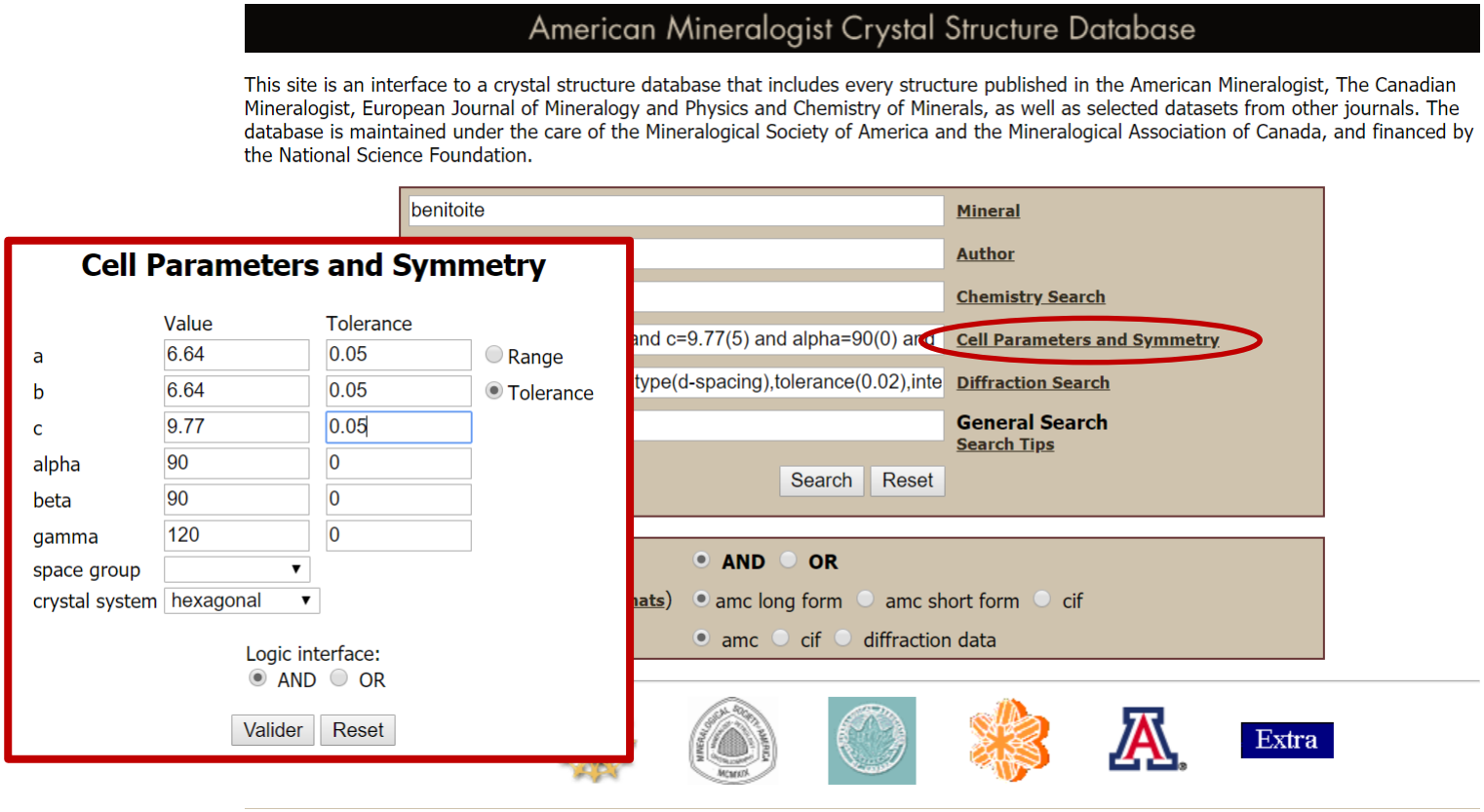
http://rruff.geo.arizona.edu/AMS/amcsd.php

Open database : AMCSD example



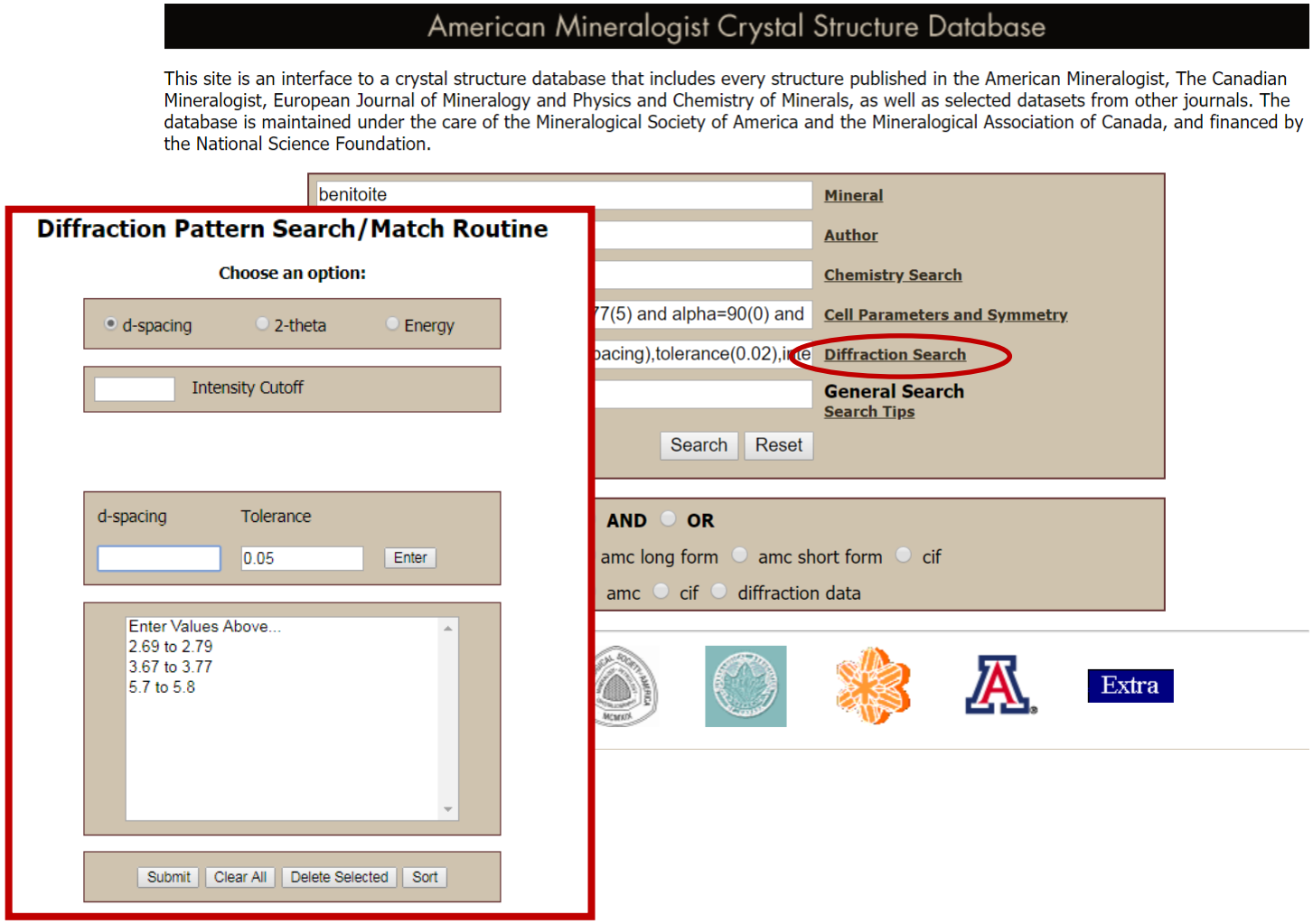
http://rruff.geo.arizona.edu/AMS/amcsd.php

Open database : AMCSD example



http://rruff.geo.arizona.edu/AMS/amcsd.php

Open database : AMCSD example



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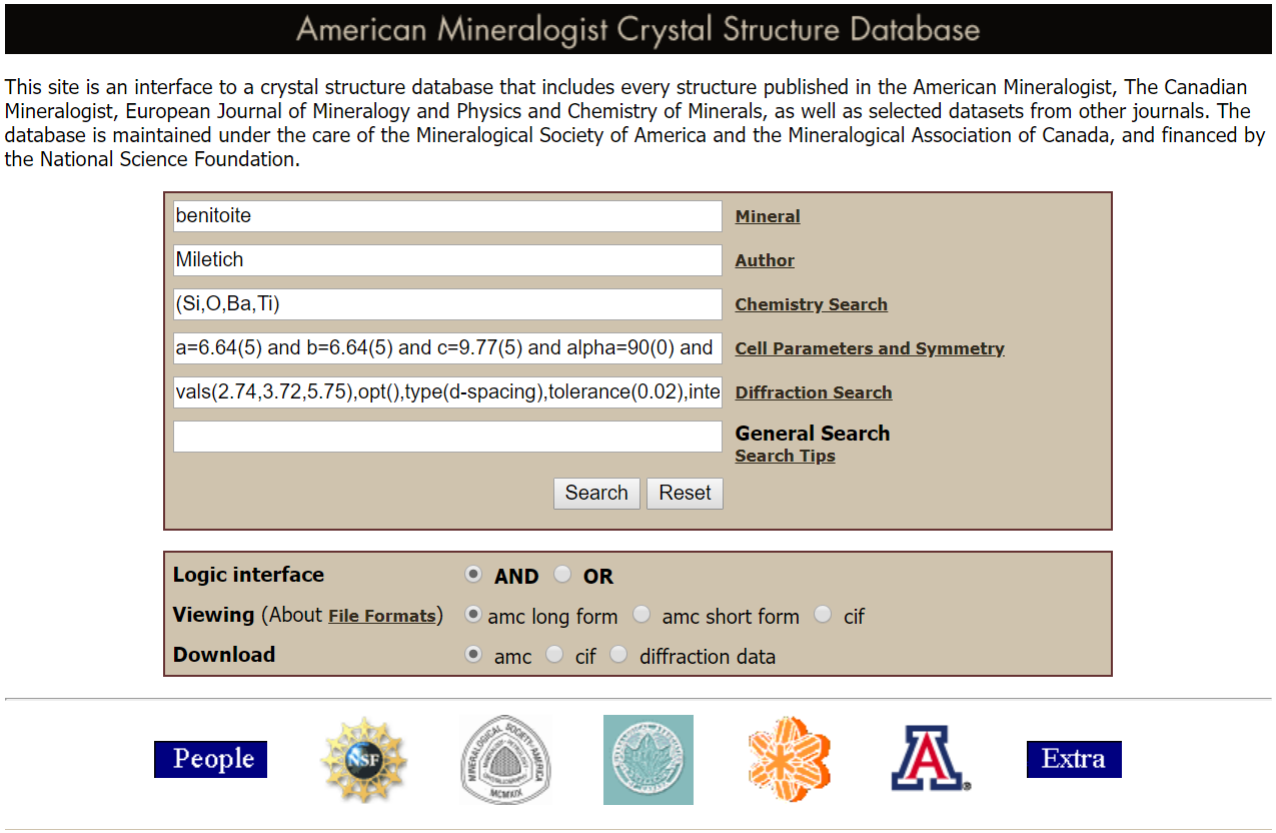
Open database : AMCSD example



http://rruff.geo.arizona.edu/AMS/amcsd.php

Open database : AMCSD example

American Mineralogist Crystal Structure Database

1 matching records for this search.

Benitoite

Hejny C, Miletich R, Jasser A, Schouwink P, Crichton W, Kahlenberg V
American Mineralogist 97 (2012) 1749-1763
Second-order P6c2-P31c transition and structural crystallography of
the cyclosilicate benitoite, $BaTiSi_3O_9$, at high pressure
Note: P = 0.0001 GPa
Locality: San Benito, California, USA
_database_code_amcsd 0019506
6.6430 6.6430 9.7660 90 90 120 P-6c2

atom	x	y	z	Uiso
Ba	2/3	1/3	0	.0074
Ti	1/3	2/3	0	.0032
Si	.0705	.7817	.25	.0014
O1	.809	.745	.25	.0024
O2	.0862	.6578	.3877	.0039

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Cif file

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'Miletich R'
'Jasser A'
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'Crichton W'
'Kahlenberg V'
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_journal_volume 97
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 the cyclosilicate benitoite, BaTiSi3O9, at high pressure
 Note: P = 0.0001 GPa
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  'x,x-y,-z'
  '-x+y,-x,1/2-z'
  '-y,-x,1/2+z'
```

http://rruff.geo.arizona.edu/AMS/amcsd.php

Open database : AMCSD example

American Mineralogist Crystal Structure Database

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Benitoite

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Total number of retrieved datasets: **1**
View in **amclongform**, download in **amc**

Diffraction data

Benitoite
Hejny C, Miletich R, Jasser A, Schouwink P, Crichton W, Kahlenberg V
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Note: P = 0.0001 GPa
Locality: San Benito, California, USA
_database_code_amcsd 0019506

CELL PARAMETERS: 6.6430 6.6430 9.7660 90.000 90.000 120.000
SPACE GROUP: P-6c2
X-RAY WAVELENGTH: 1.541838
MAX. ABS. INTENSITY / VOLUME**2: 52.45539891

2-THETA	INTENSITY	D-SPACING	H	K	L	Multiplicity
15.40	25.74	5.7530	1	0	0	3
18.17	3.06	4.8830	0	0	2	2
23.90	100.00	3.7228	1	0	2	6
26.84	16.01	3.3215	1	1	0	6
28.38	11.86	3.1446	1	1	1	12
31.09	28.17	2.8765	2	0	0	3
32.60	81.12	2.7464	1	1	2	12
36.25	5.21	2.4784	2	0	2	6
36.81	10.09	2.4415	0	0	4	2
40.12	9.02	2.2475	1	0	4	6
41.53	18.58	2.1744	2	1	0	6
42.60	6.50	2.1225	2	1	1	12
45.67	13.16	1.9864	2	1	2	12
46.14	17.01	1.9672	1	1	4	12
47.41	11.93	1.9177	3	0	0	3
48.93	16.23	1.8614	2	0	4	6
50.47	2.18	1.8082	2	1	3	12
51.18	14.35	1.7850	3	0	2	6
55.32	4.88	1.6608	2	2	0	6
56.69	12.34	1.6238	2	1	4	12
57.78	1.75	1.5956	3	1	0	6
58.62	3.13	1.5747	3	1	1	12
58.72	7.09	1.5723	2	2	2	12

http://rruff.geo.arizona.edu/AMS/amcsd.php

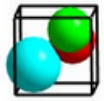
: just an other base in the land ?

Open-access collection of crystal structures of organic, inorganic, metal-organics compounds and minerals, excluding biopolymers.

Including data and software from CrystalEye, developed by Nick Day at the department of Chemistry, the University of Cambridge under supervision of Peter Murray-Rust.

All data on this site have been placed in the public domain by the contributors.

Currently there are **394494** entries in the COD.
Latest deposited structure: 4033564 on **2018-05-17** at **23:20:30 UTC**



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Robert T. Downs, Saulius Gražulis, Werner Kaminsky, Armel Le Bail, Luca Lutterotti,
Yoshitaka Matsushita, Peter Moeck, Peter Murray-Rust, Miguel Quirós Olozábal,
Hareesh Rajan, Alexandre F.T. Yokochi

If you find bugs in COD or have any feedback, please contact us at
cod-bugs@ibt.lt

Acknowledgements

http://www.crystallography.net/cod/index.php

: just an other base in the land ?

Open-access collection of crystal structures of organic, inorganic, metal-organics compounds and minerals, excluding biopolymers.

Including data and software from CrystalEye, developed by Nick Day at the department of Chemistry, the University of Cambridge under supervision of Peter Murray-Rust.

All data on this site have been placed in the public domain by the contributors.

Currently there are **394494** entries in the COD.
Latest deposited structure: 4033564 on **2018-05-17** at **23:20:30 UTC**

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- **Powder identification**
- **Source for computational material science** *Microporous and Mesoporous Materials (2013), 165: 32–39*
- **Used as source for 3D printed models for education** *J. Mater. Edu. (2014), 77–96*
- **SOLSA project : mineral identification in mines in real time**

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In future : store larger files such as diffraction images

http://www.crystallography.net/cod/index.php

The 

Idea of a consortium of independent researchers from different countries driven by the desire to provide a free tool to preserve data and make them available to the "world"

- Web

  www.crystallography.net/cod

- Advisory board

  Saulius Gražulis, Andrius Merkys, Antanas Vaitkus, Armel Le Bail, Daniel Chateigner , Henry Pilliere, Robert T. Downs, Luca Lutterotti, Peter Moeck, Peter Murray-Rust, Miguel Quirós Olozábal, Werner Kaminsky

The project has recently received funding from "European Union's Horizon 2020 research and innovation program "

The COD project

- Why set up a database containing all the crystallography data?

  - ✓ Escape the current situation with fragmented databases (organic / inorganic materials ...)
  - ✓ Prevent monopoly and dependency on private databases

- What are the needs to set up this database?

  - ✓ a small "committed" scientific team with experience on databases and a software to coordinate the project.
  - ✓ A free software to maintain the base, to evaluate the data, to make computations on the data (calculation of "powder" diffraction diagrams ...) and to carry out research in the database
  - ✓ You ! And your CIF !!!

Crystallography Open Database : basic search

COD Home

- Home
- What's new?

Accessing COD Data

- Browse
- Search
- Search by structural formula
  - JSME search
  - JCP search

Add Your Data

- Deposit your data
- Manage depositions
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Documentation

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text (1 or 2 words)	baptiste
journal	inorganic chemistry
year	
volume	
issue	
DOI	
Z (min, max)	
Z' (min, max)	
chemical formula (in Hill notation)	
1 to 8 elements	Li B O
NOT these elements	
volume min and max	
number of distinct elements min and max	3 3
filters	☐ has F_{obs} ☐ include duplicates ☐ include structures with errors ☐ include theoretical structures
Reset	Send

a (min - max)		
b		
c		
alpha	90	90
beta	90	90
gamma	90	90
filters	☐ has F_{obs} ☐ include duplicates ☐ include structures with errors ☐ include theoretical structures	
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b		
c		
alpha	90	90
beta	90	90
gamma	90	90
filters	☐ has F_{obs} ☐ include duplicates ☐ include structures with errors ☐ include theoretical structures	
Reset	Send	

result

COD ID ▲	Links	Formula ▲	Space group ▲	Cell parameters	Cell volume ▲	Bibliography
4338443	CIF	B4 Li6 O9	P 1 21/n 1	3.31913; 23.361; 9.1582 90; 92.65; 90	709.35	Rousse, Gwenaëlle; Baptiste, Benoît; Lelong, Gérald Crystal Structures of Li6B4O9 and Li3B11O18 and Application of the Dimensional Reduction Formalism to Lithium Borates. *Inorganic chemistry*, **2014**, *53*, 6034-6041
4338444	CIF	B11 Li3 O18	P 1 21/c 1	17.7607; 7.7737; 9.6731 90; 100.906; 90	1311.41	Rousse, Gwenaëlle; Baptiste, Benoît; Lelong, Gérald Crystal Structures of Li6B4O9 and Li3B11O18 and Application of the Dimensional Reduction Formalism to Lithium Borates. *Inorganic chemistry*, **2014**, *53*, 6034-6041

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COD Home
- Home
- What's new?

Accessing COD Data
- Browse
- Search
- Search by structural formula
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Add Your Data
- Deposit your data
- Manage depositions
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Documentation
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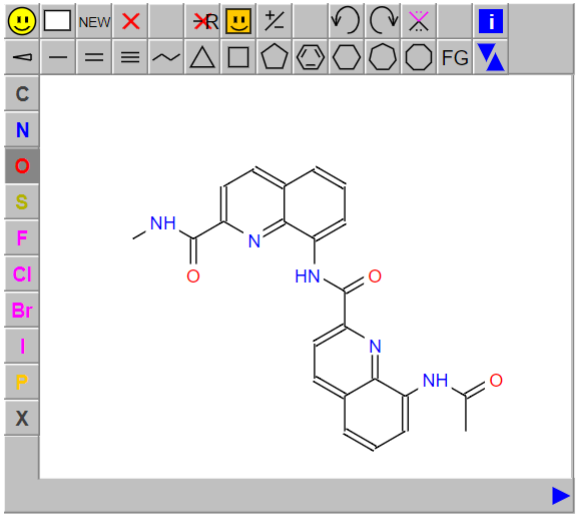
Draw a structure or a fragment to search in COD



Exact match ☐

Search

Use JME search

Note: substructure search by SMARTS is currently available in a subset of the COD containing 162172 structures.

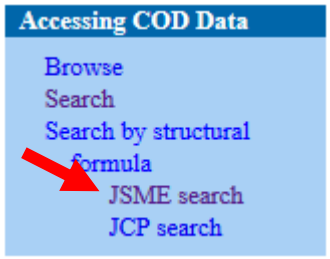
Just 1 result ?

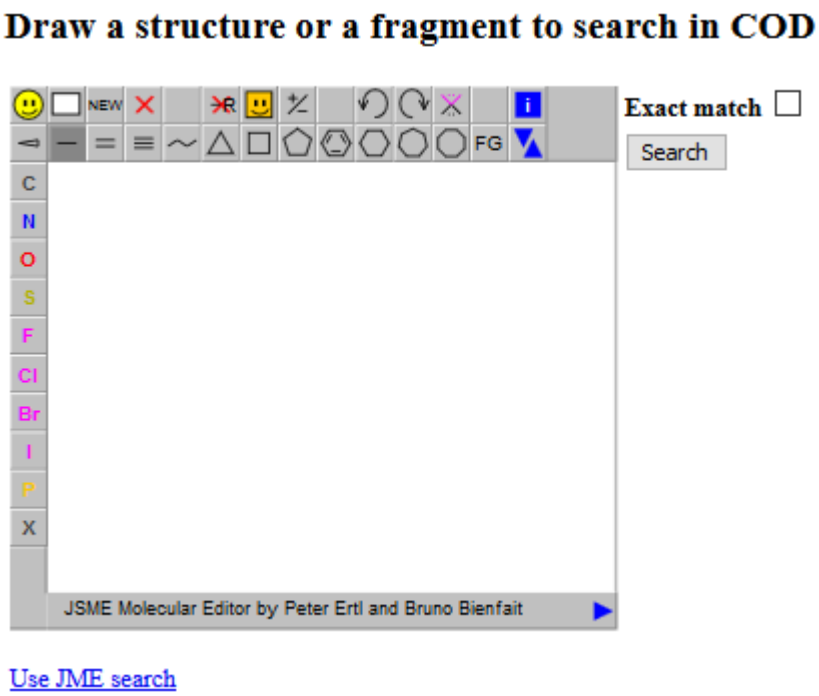
COD ID ▲	Links	Formula ▲	Space group ▲	Cell parameters	Cell volume ▲	Bibliography
4120055	CIF HKL	C146 H180 N20 O24 Si	P -1	15.9947; 18.9533; 29.923 97.74; 92.316; 112.924	8235.7	Mayumi Kudo; Victor Maurizot; Brice Kauffmann; Aya Tanatani; Ivan Huc Folding of a Linear Array of α-Amino Acids within a Helical Aromatic Oligoamide Frame *Journal of the American Chemical Society*, **2013**, *135*, 9628-9631

http://www.crystallography.net/cod/

To be improved…

Live search …





http://www.crystallography.net/cod/jsme_search.html

COD: also compatible with search and match programs

COD Home

Home
What's new?

Accessing COD Data

Browse
Search
Search by structural formula
JSME search
JCP search

Add Your Data

Deposit your data
Manage depositions
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Documentation

COD Wiki
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What's New?

- **September 2016**: Thomas Sander (Actelion) has released a new version of the DataWarrior program which now allows to carry out structure search queries in the organic subset of the COD.
- **July 2016**: A new release of the COD-based search-match database is available from Rigaku.
- **July 2016**: A new release of the COD-based search-match database is available from PANalytical.
- **September 2015**: Thomas Sander now offers the organic part of the COD database for download on his website.
- **April 2015**: Thomas Sander from Actelion has relased the DataWarrior program as open-source!
- **November 2014**: The "FPSM method" uses a Rietveld like fitting procedure to test all possible crystal structures from the Crystallography Open Database, rank them and find the more probable in your diffraction pattern. In the end a Rietveld phase quantification is done with the phases identified. The new paper is sumitted to the J. Appl. Cryst.
- **November 2014**: The new QUALX version has been developed that can use COD data for search-match material identification.
- February 2007: Creation of the **P2D2** ; Predicted Powder Diffraction Database
  61015 entries - search-match possible with the EVA Bruker software

http://www.crystallography.net/cod/

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- Home
- What's new?

Accessing COD Data
- Browse
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- What's new?

Accessing COD Data
- Browse
- Search
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- Deposit your data
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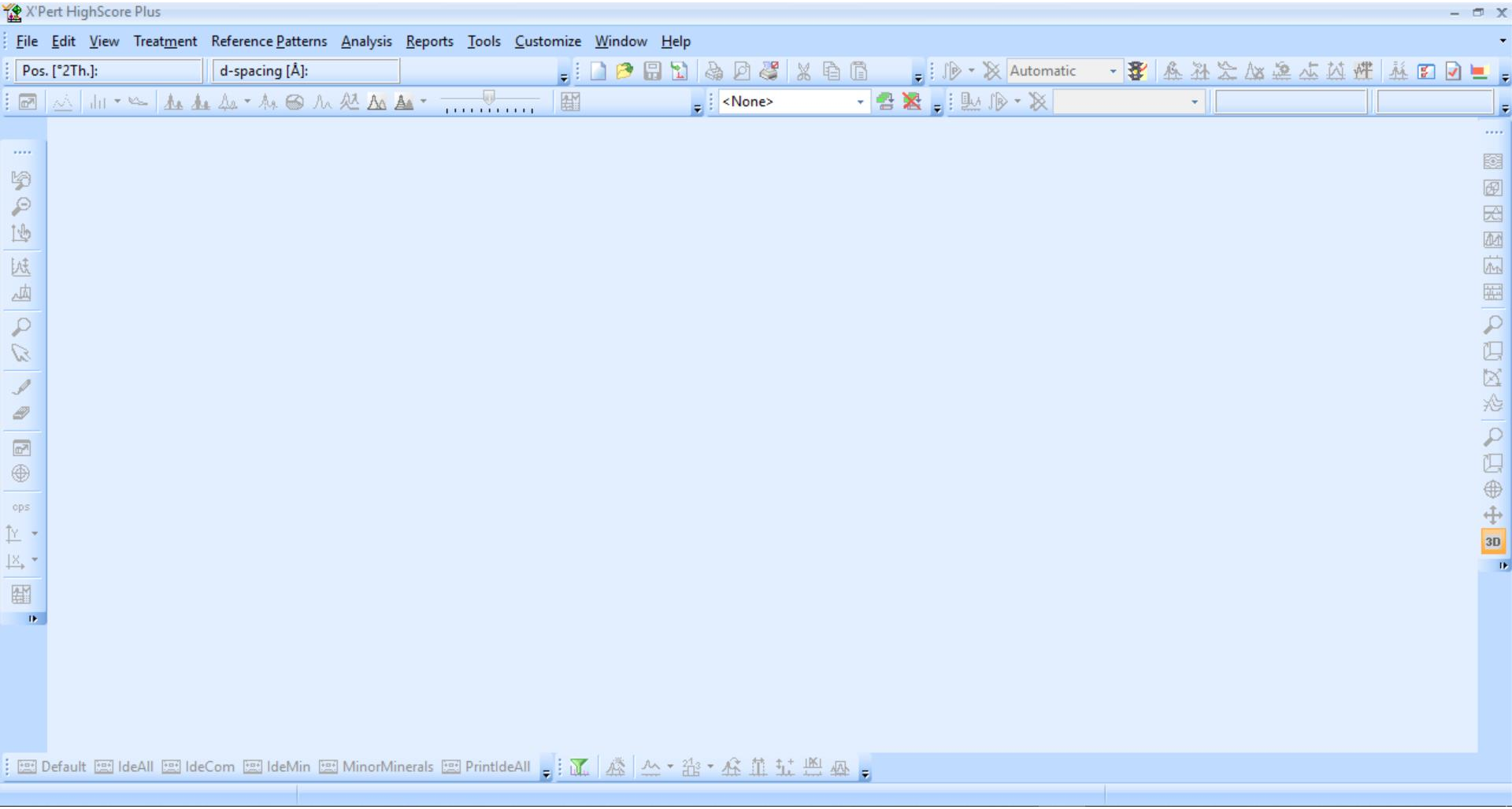
- **July 2016**: A new release of the COD-based search-match database is available from PANalytical. → HighScore(Plus)

Download the archive for your commercial or open program

Index of /cod/archives/2016/PANalytical

Name	Last modified	Size	Description
Parent Directory		-	
COD_2016_ConvHS4x.zip	2016-06-30 17:37	3.6G	
COD_Jun2016_ReadMe.rtf	2016-07-01 11:41	80K	
md5sum.dat	2016-07-01 11:50	117	
sha1sum.dat	2016-07-01 11:51	133	

Phase identification using COD with HighScore(Plus)



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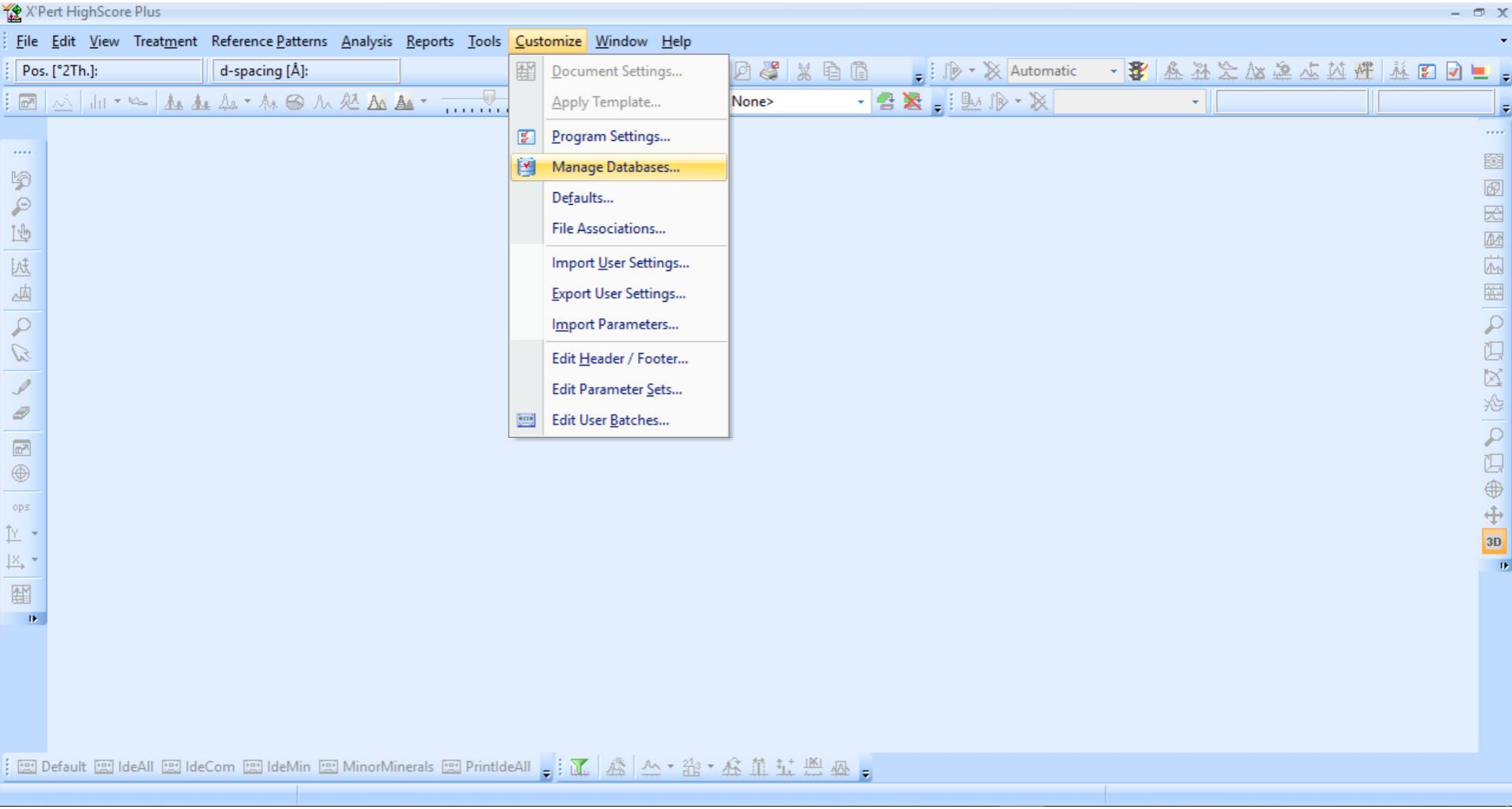

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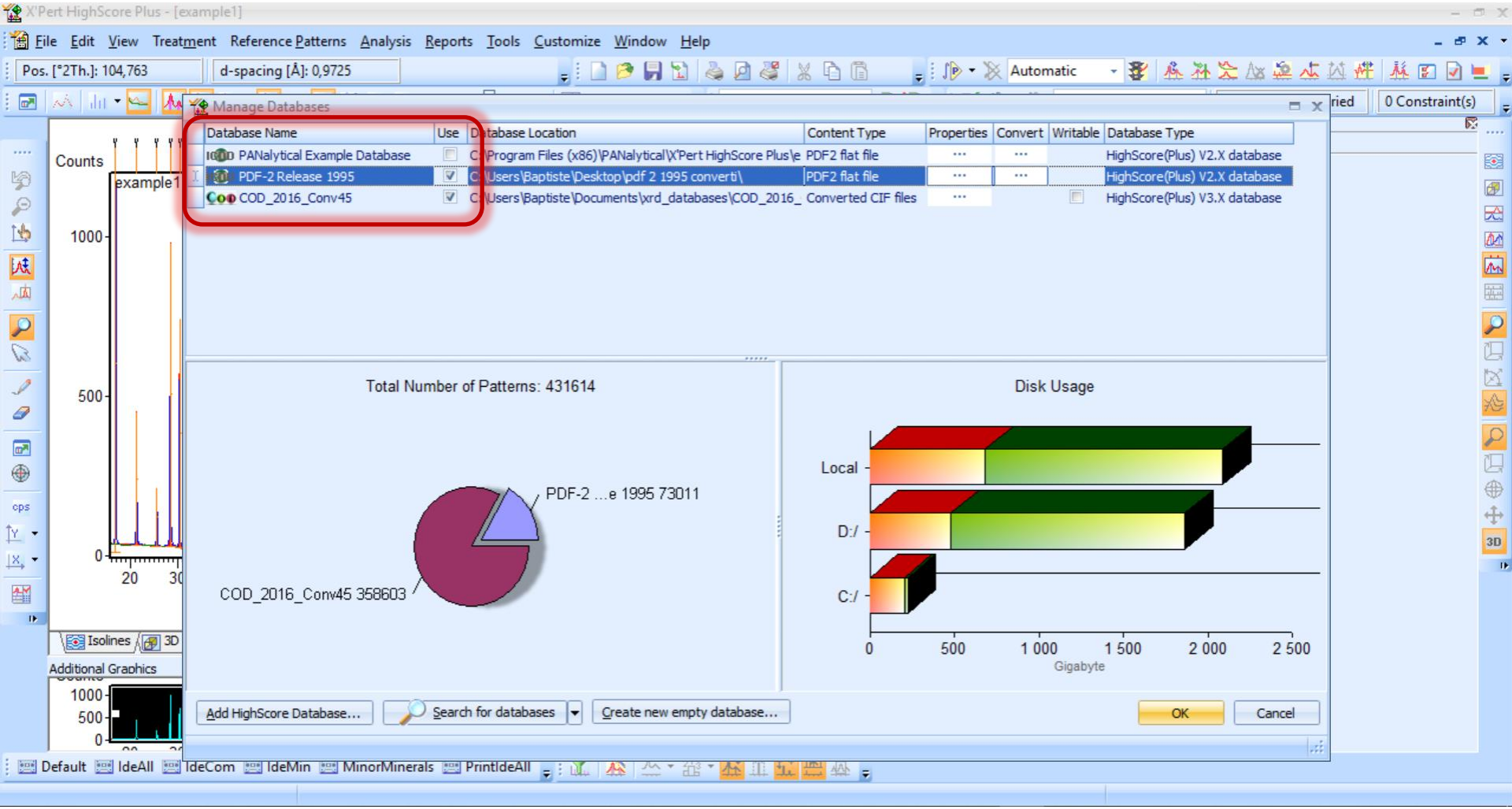
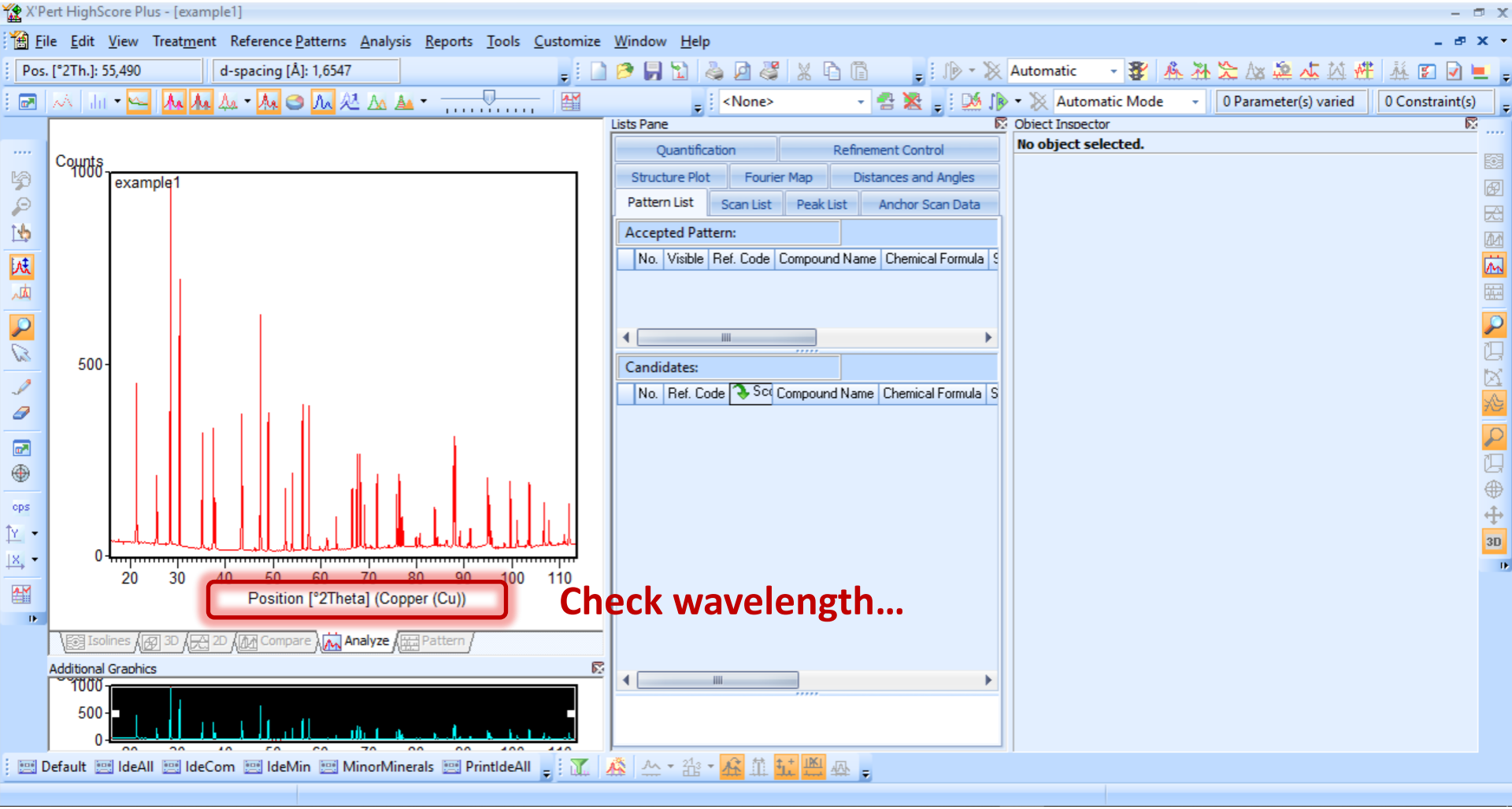


Phase identification using COD with HighScore(Plus)

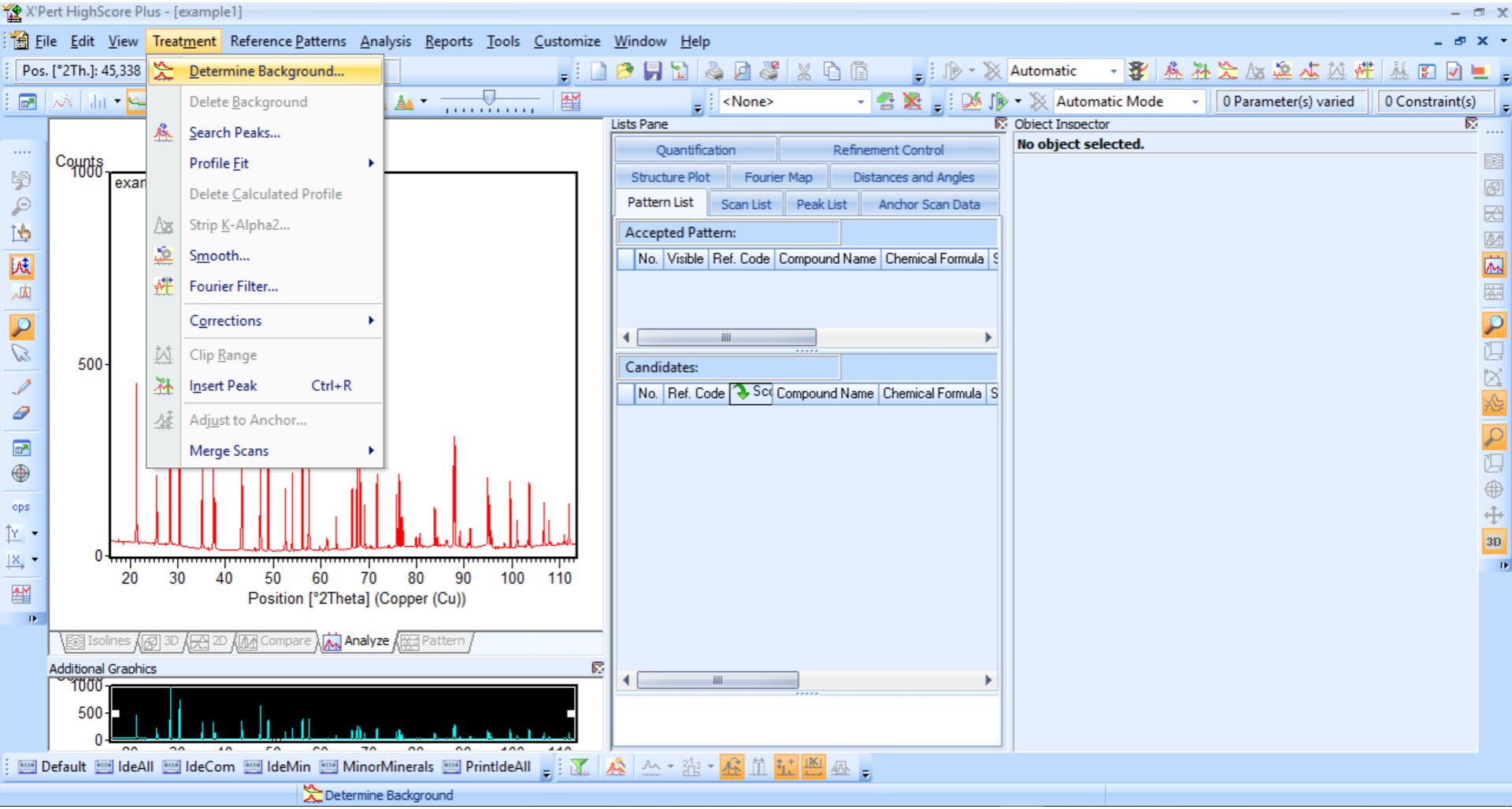
Format : .xrdml or .asc file (=.xy but must be .asc…)



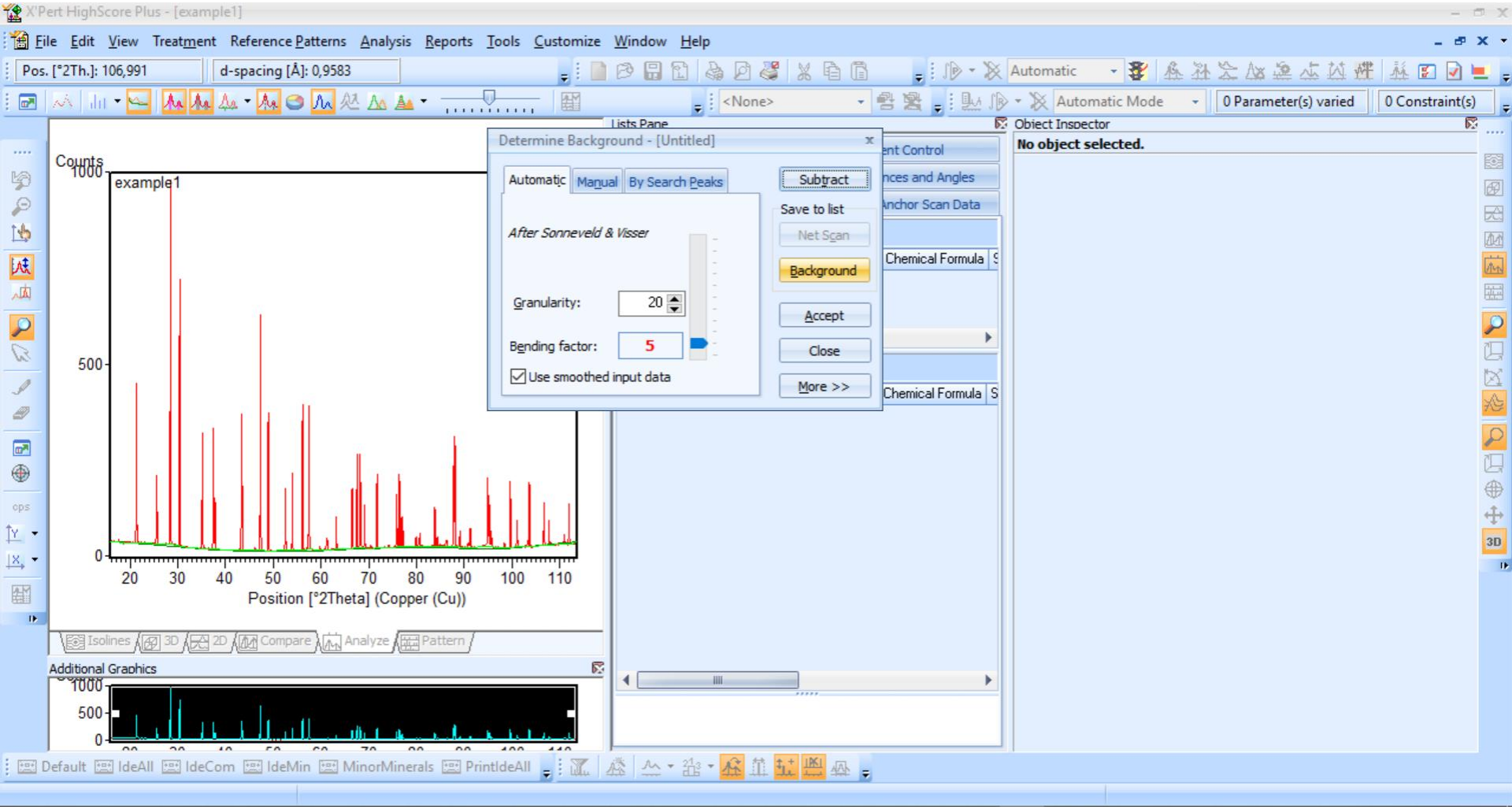
Check wavelength…

Phase identification using COD with HighScore(Plus)

Classical procedure : first model a bgd

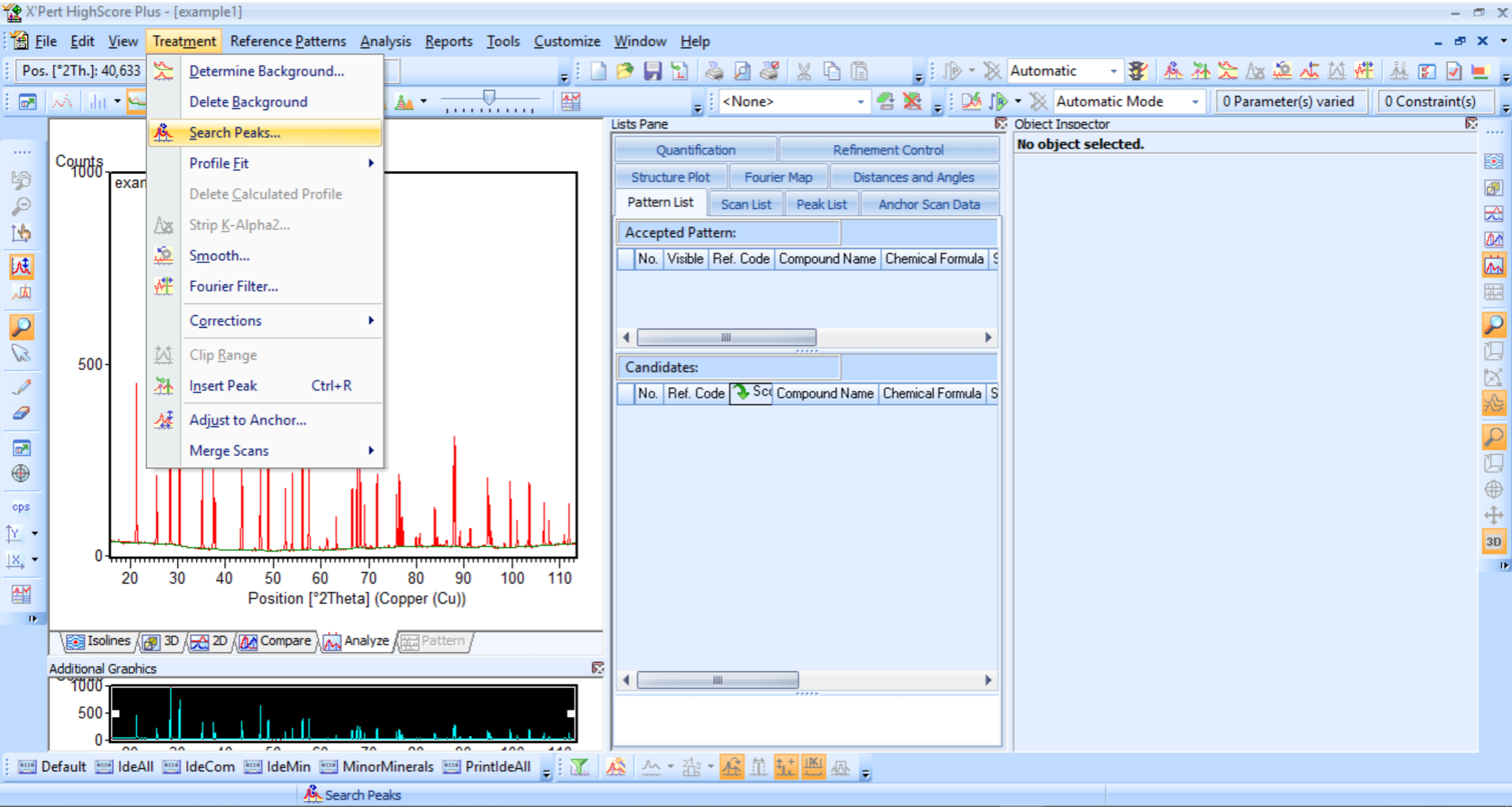


Phase identification using COD with HighScore(Plus)



Phase identification using COD with HighScore(Plus)

Classical procedure : first model a bgd and then search peak



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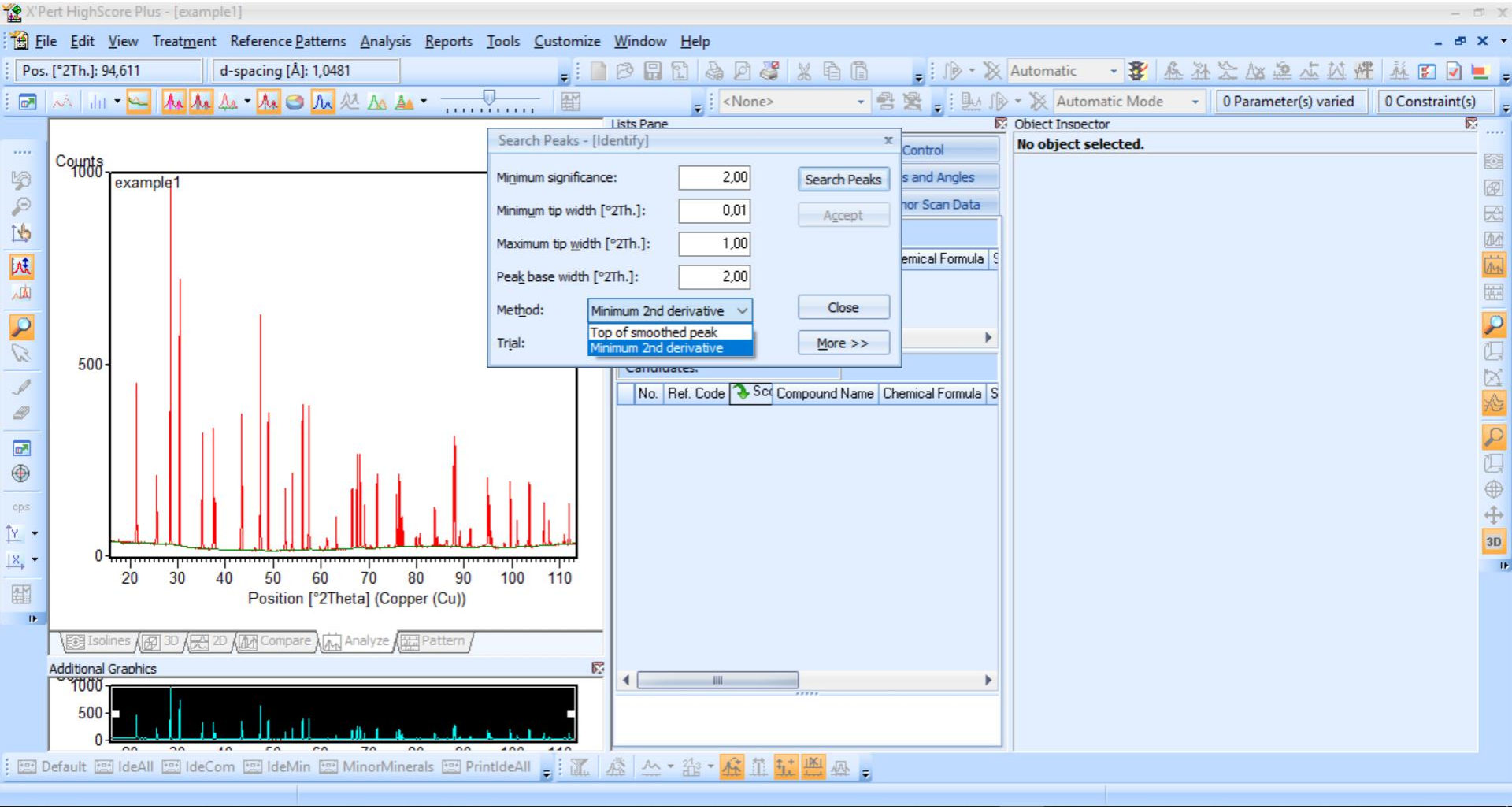

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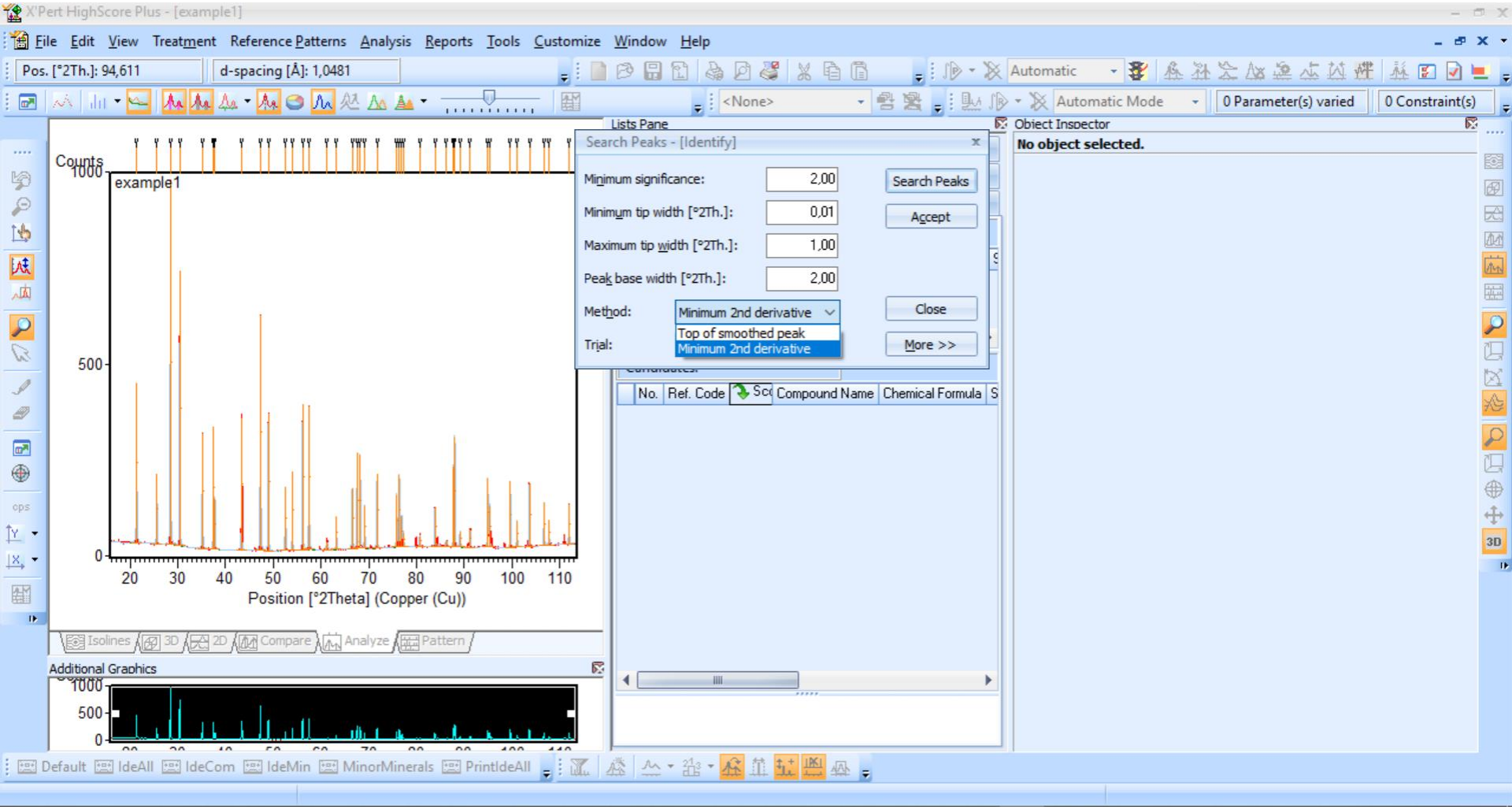
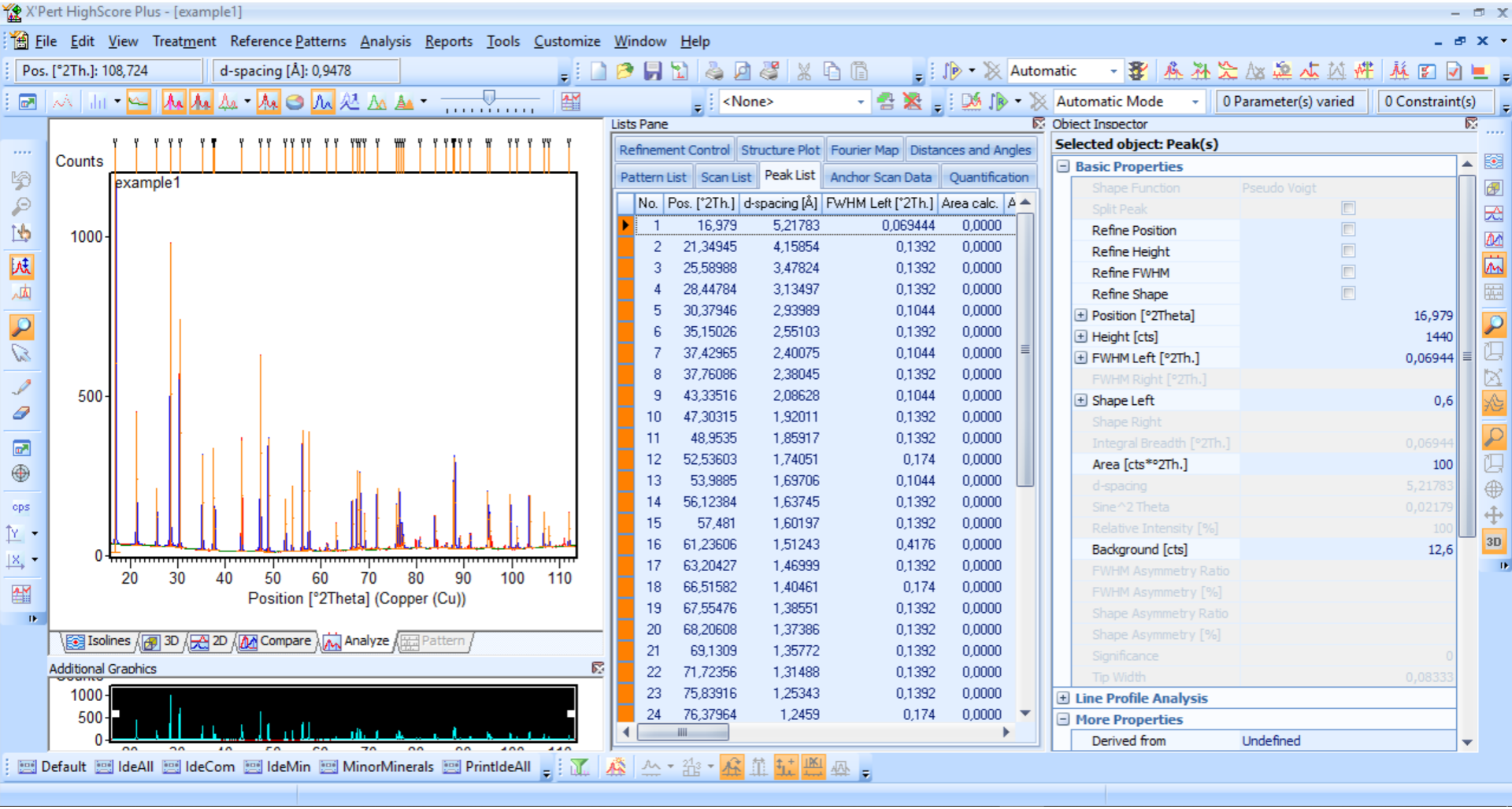


Phase identification using COD with HighScore(Plus)

Check the peak list



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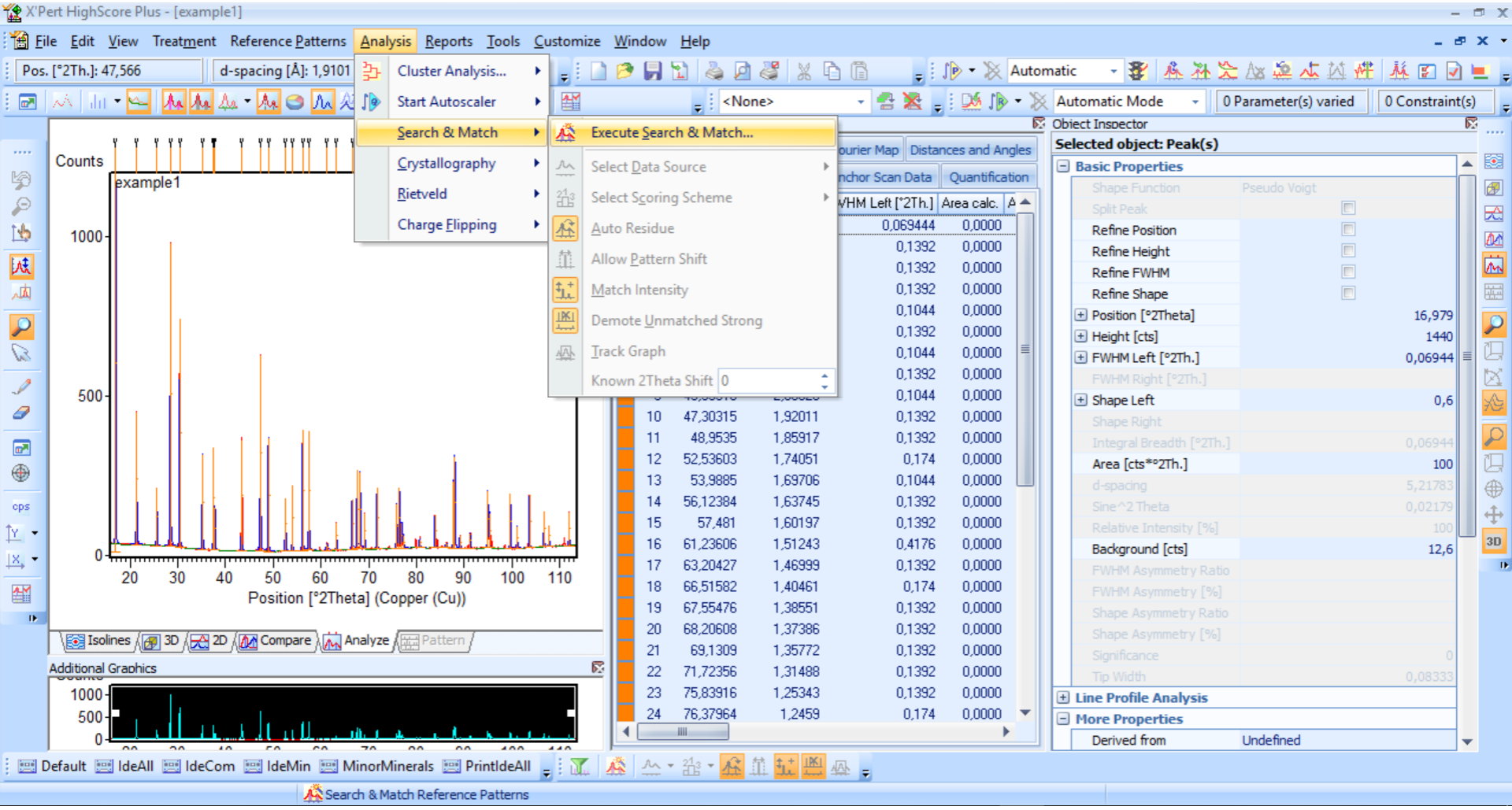

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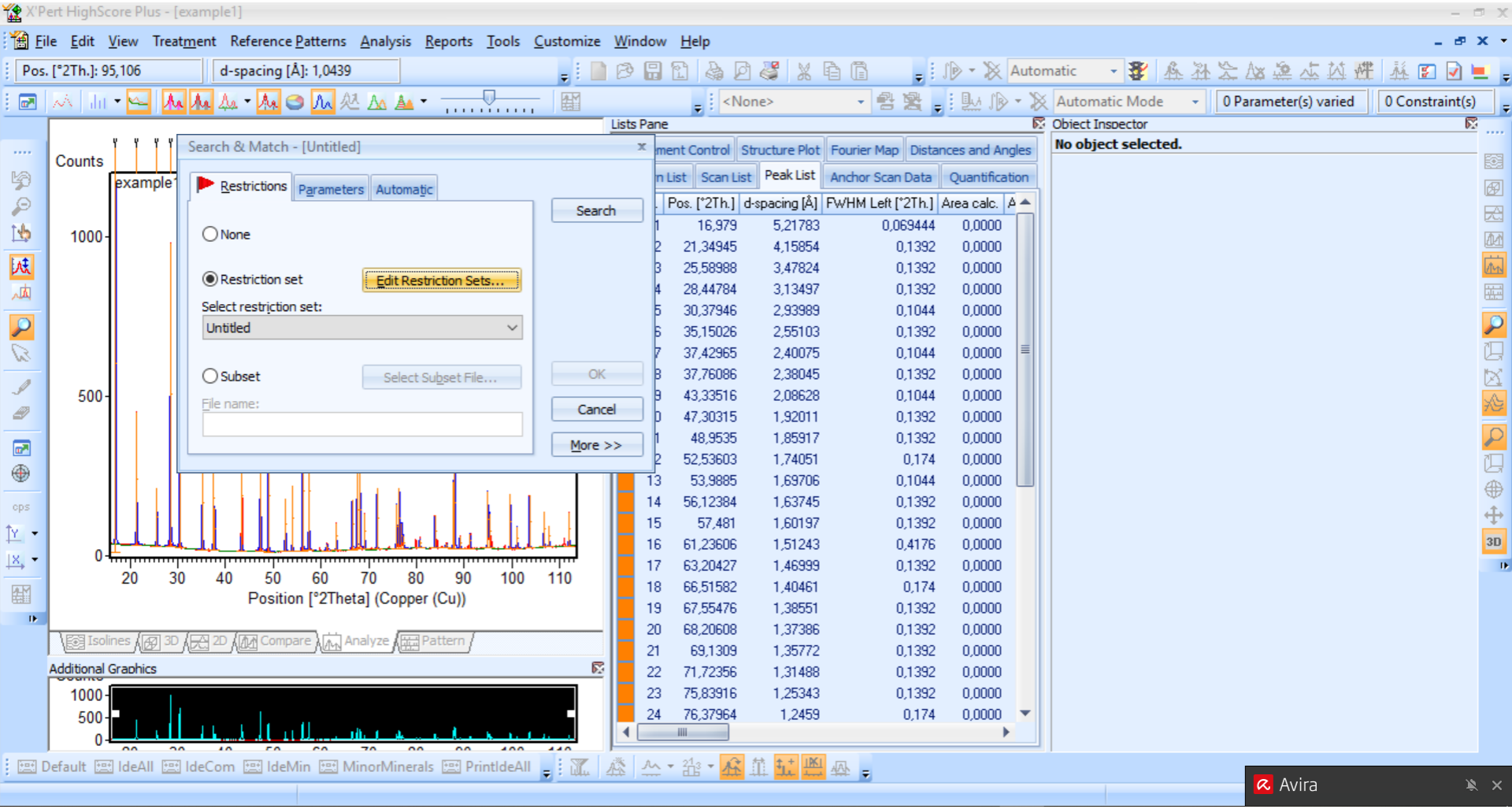
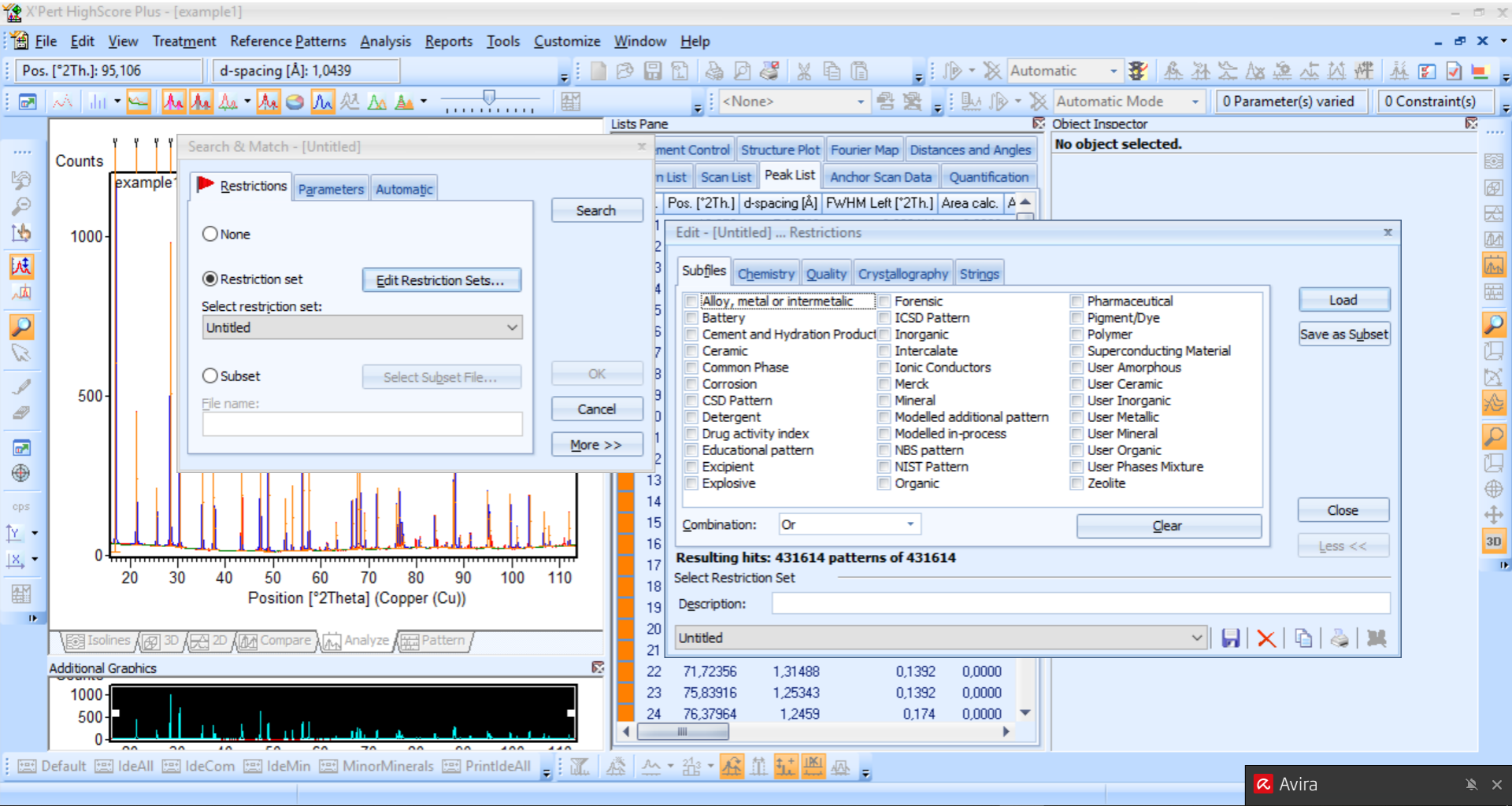


Phase identification using COD with HighScore(Plus)

Search and match with restrictions



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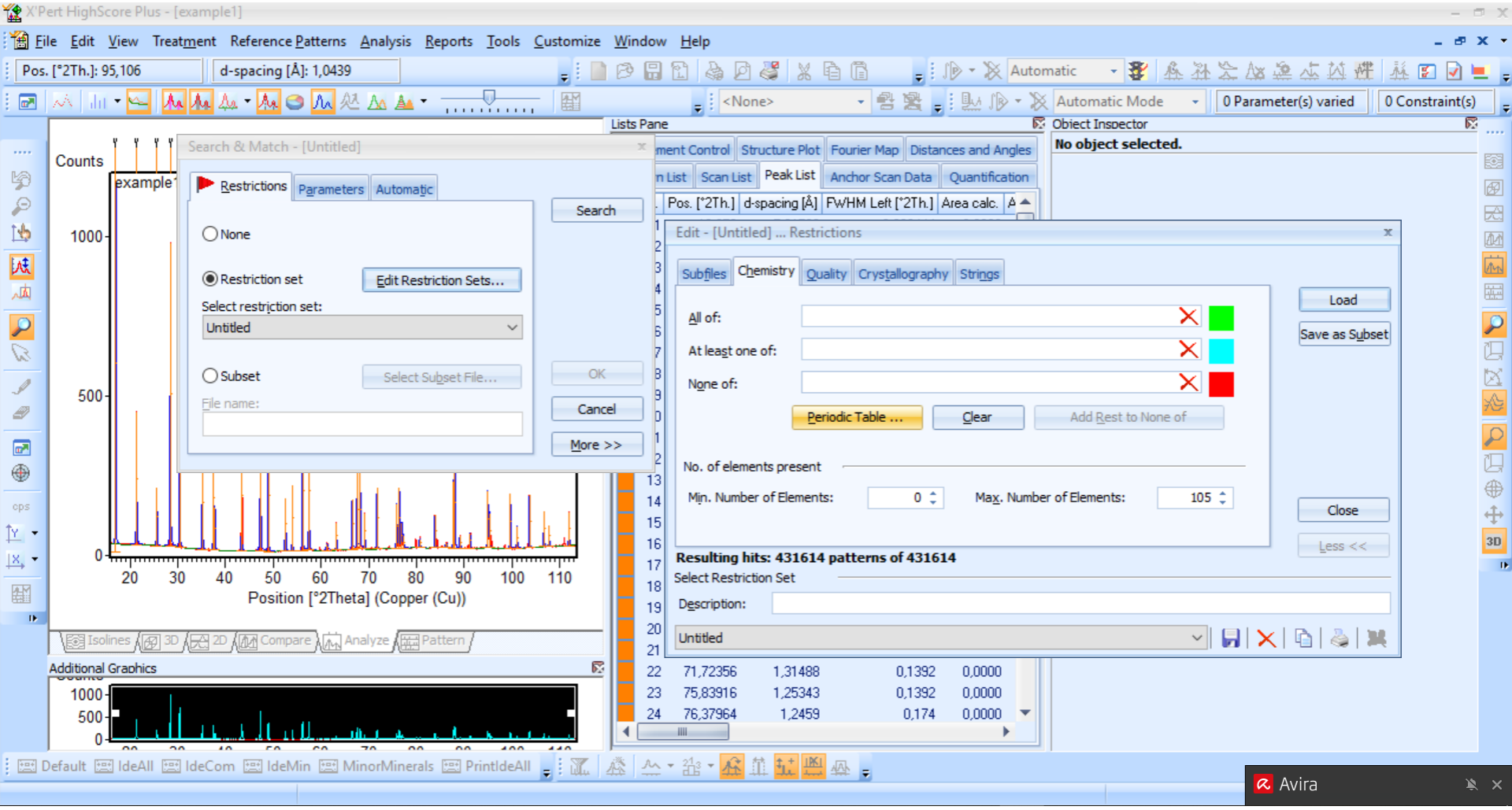

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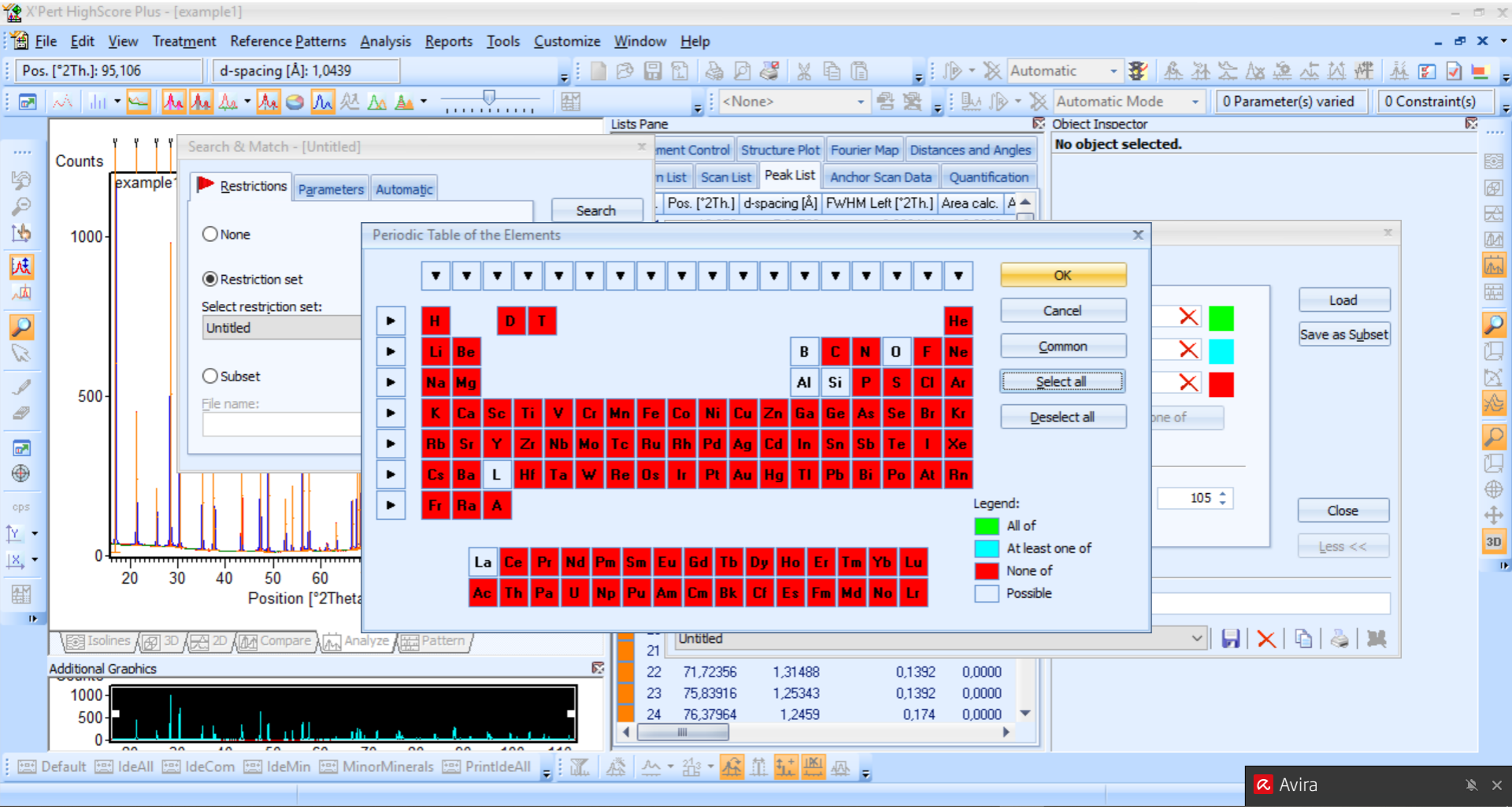

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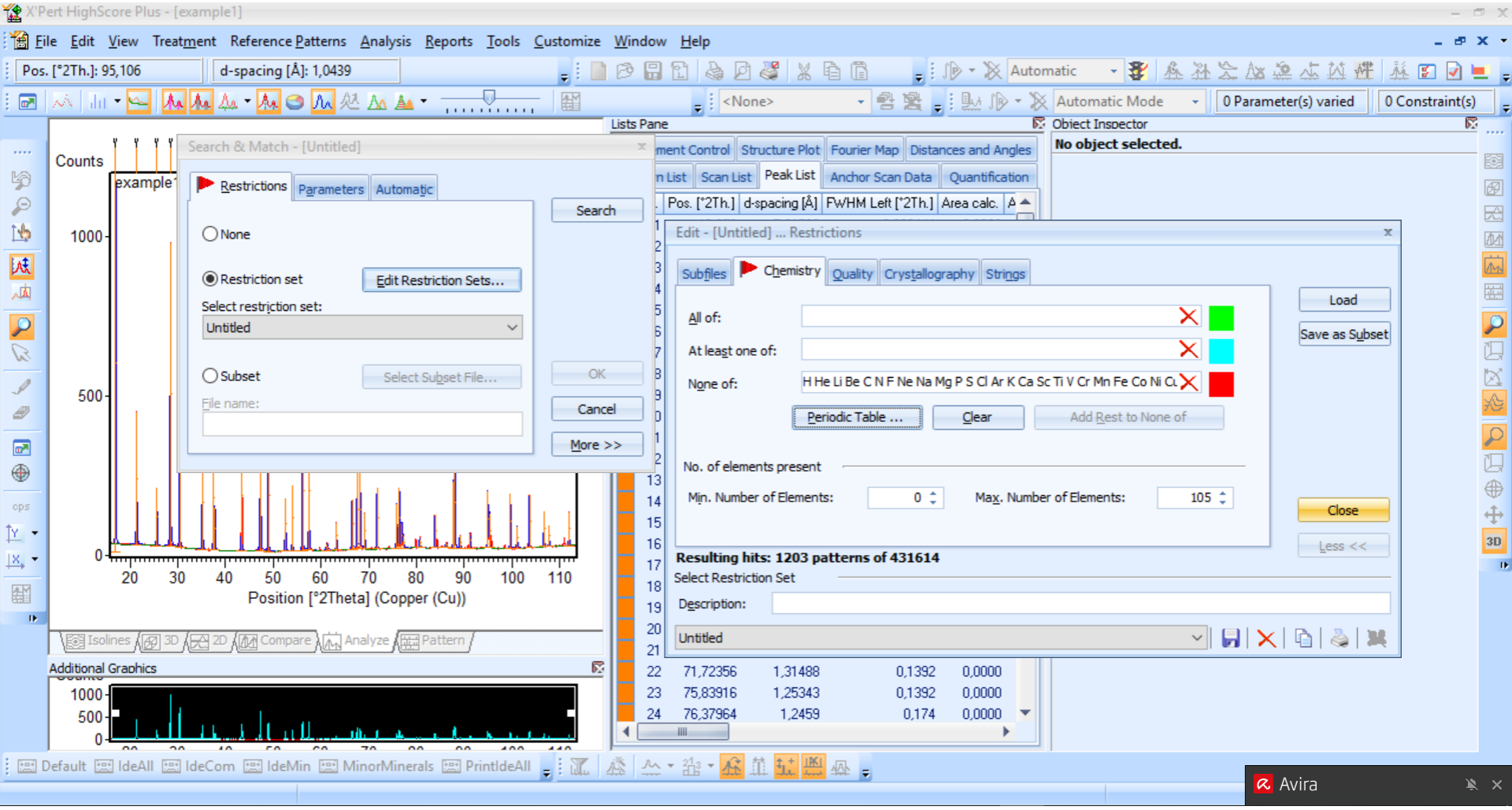

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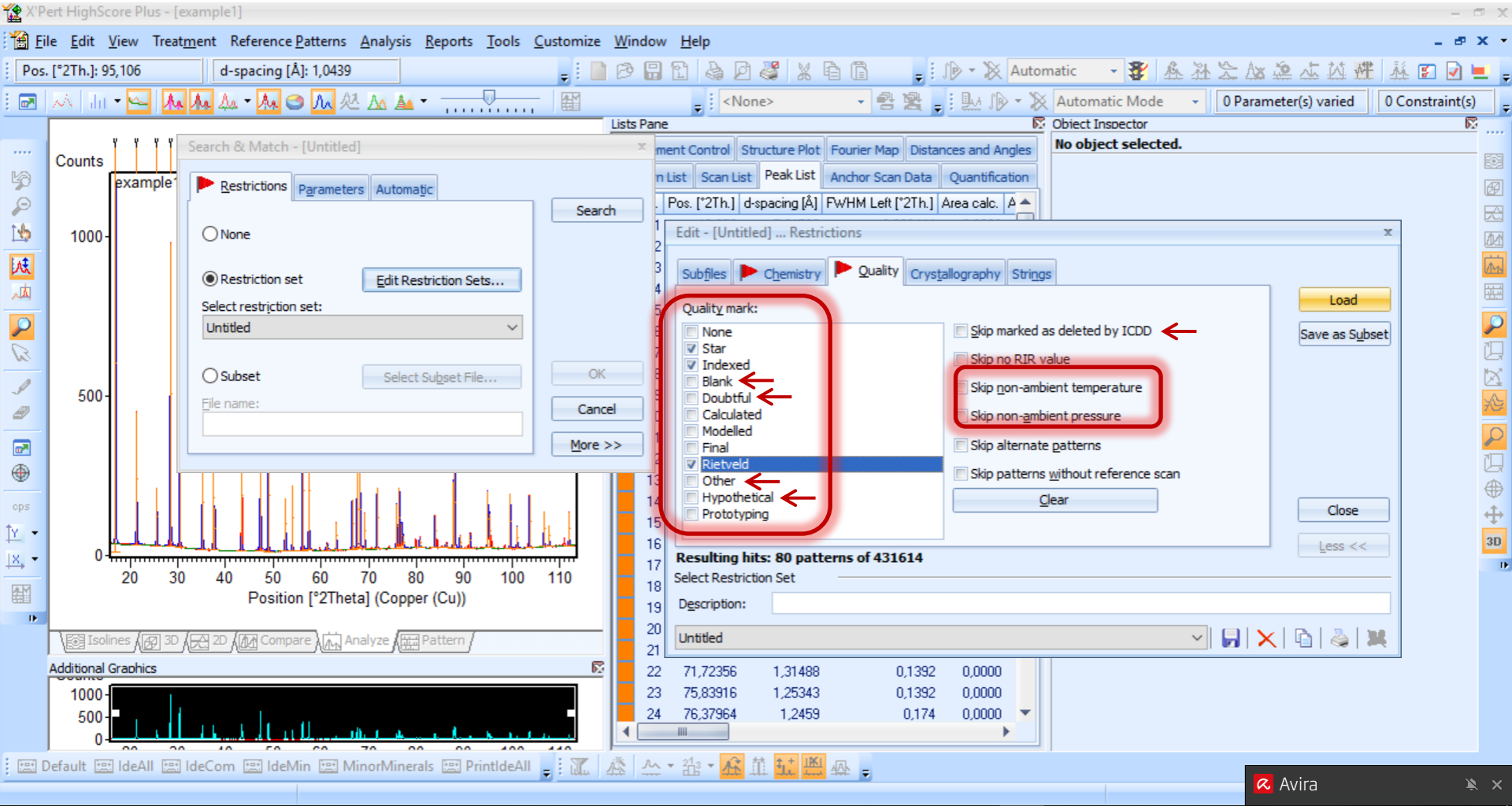

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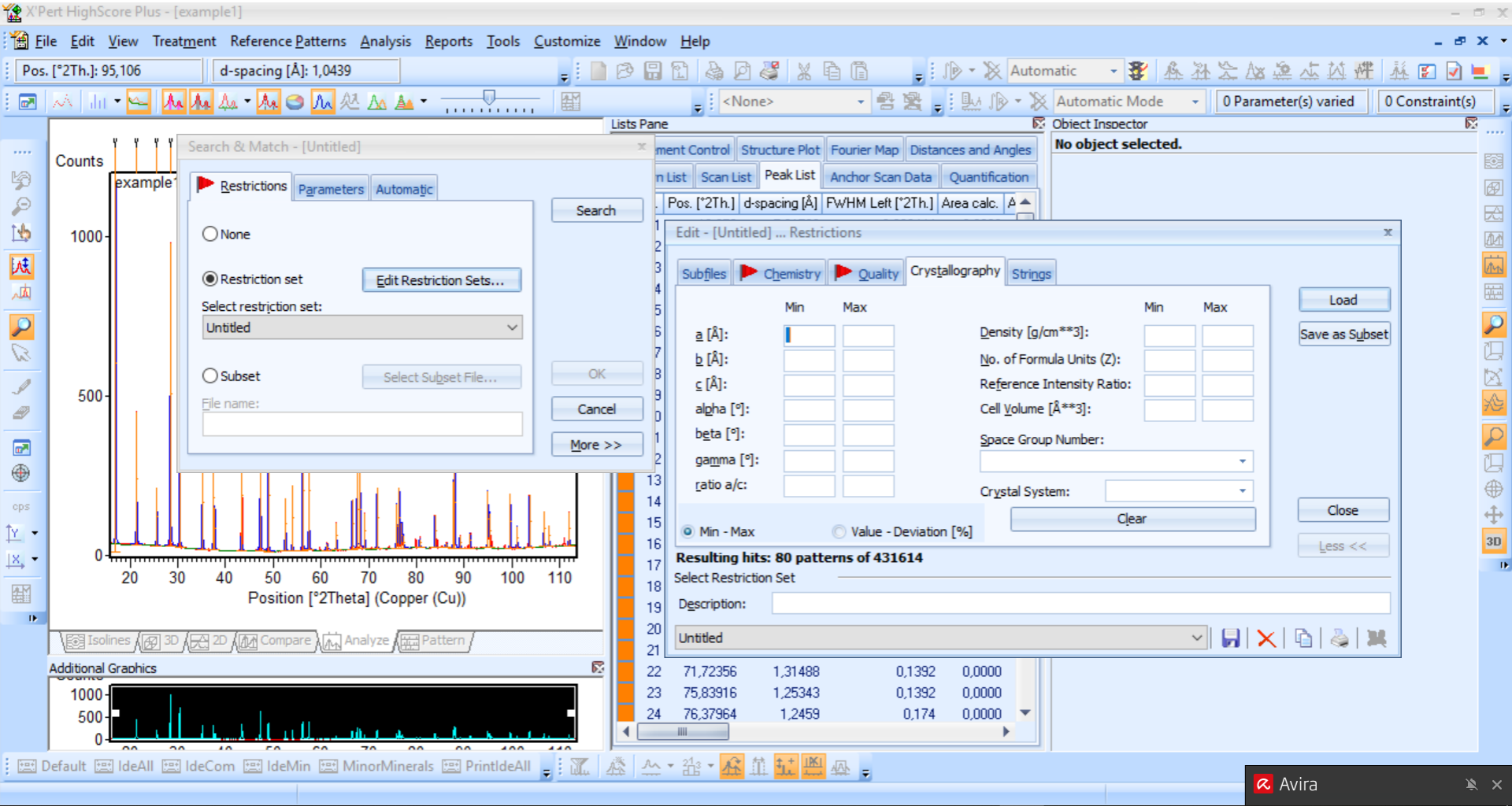

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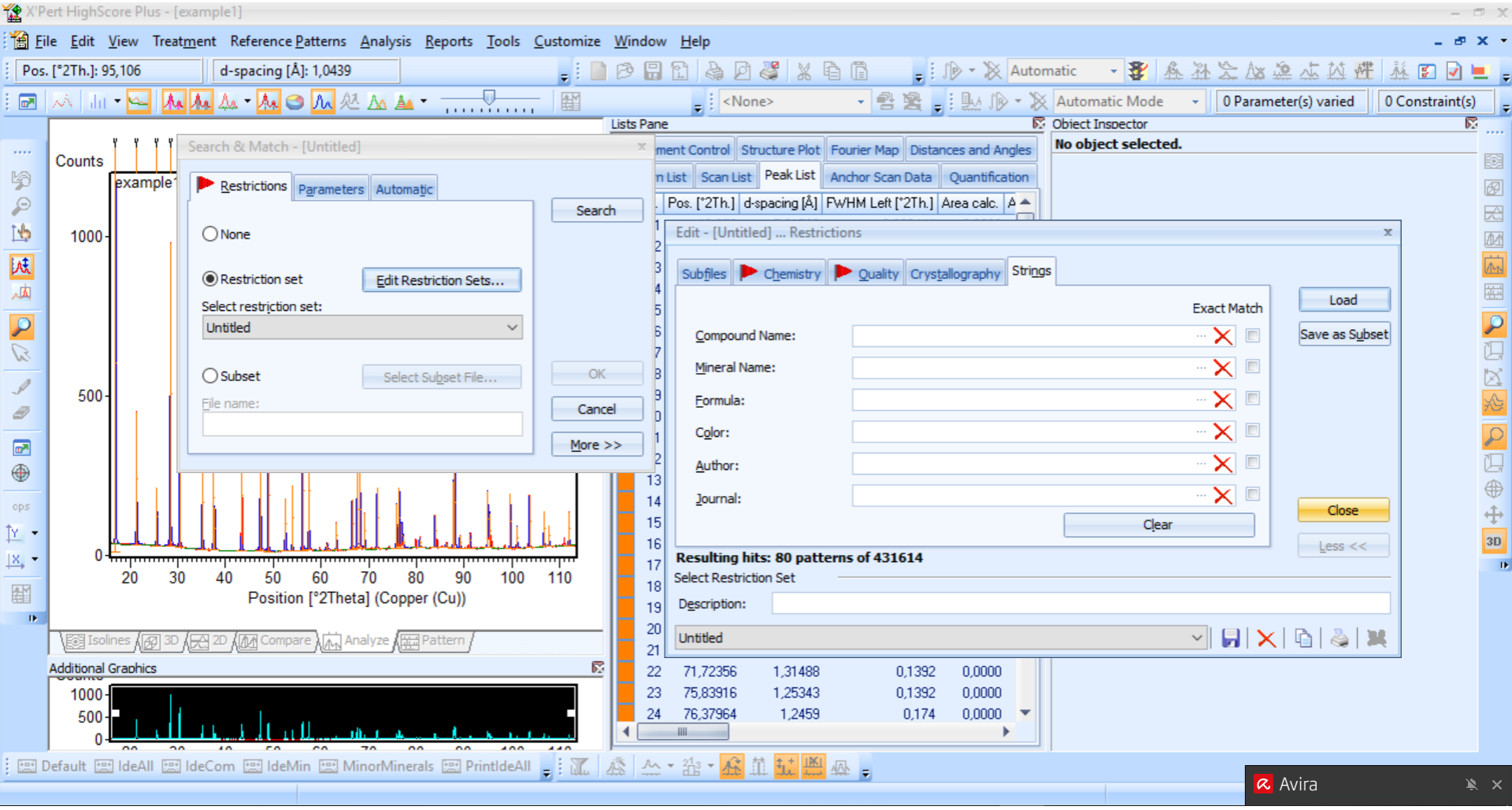

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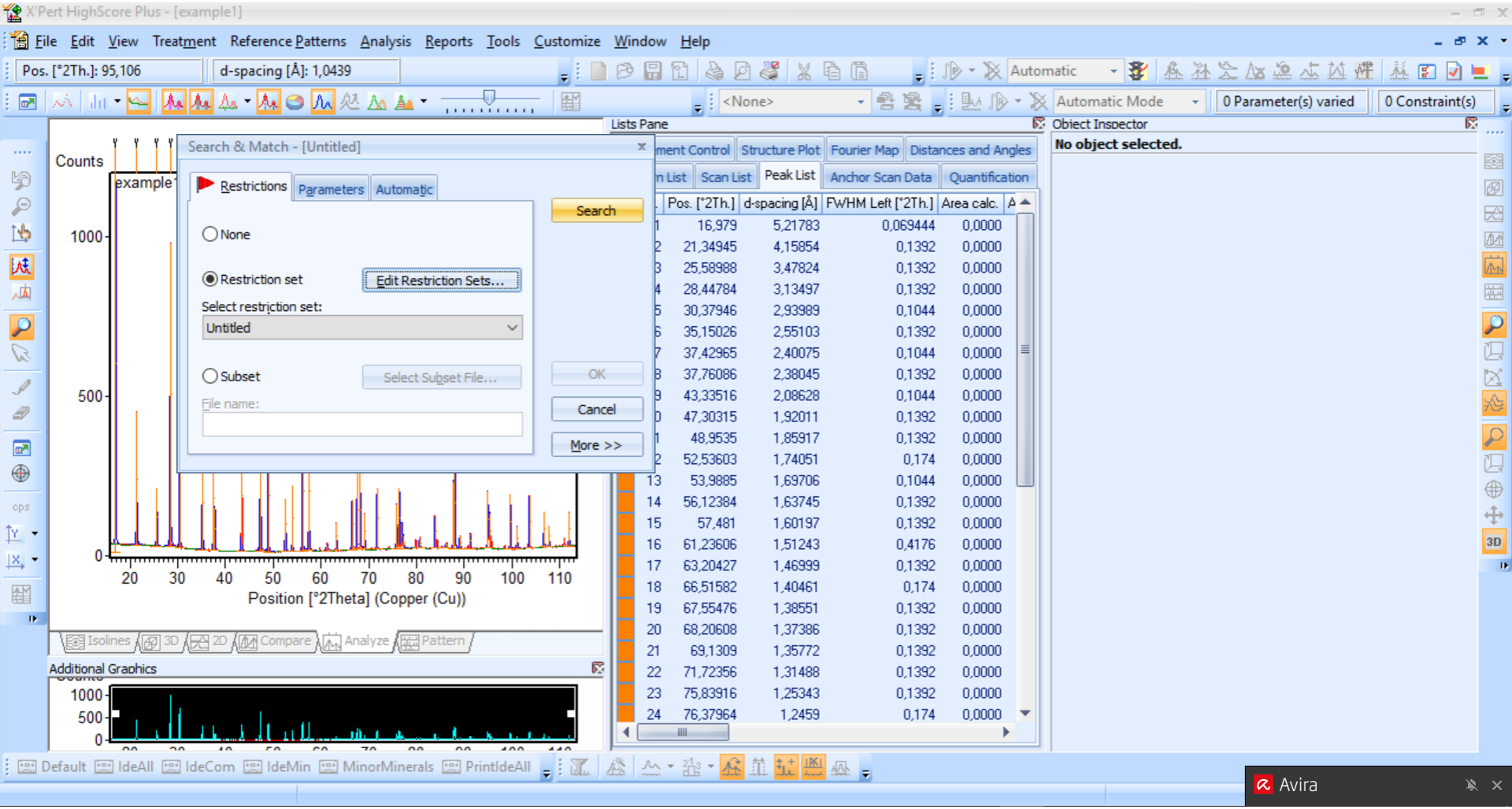

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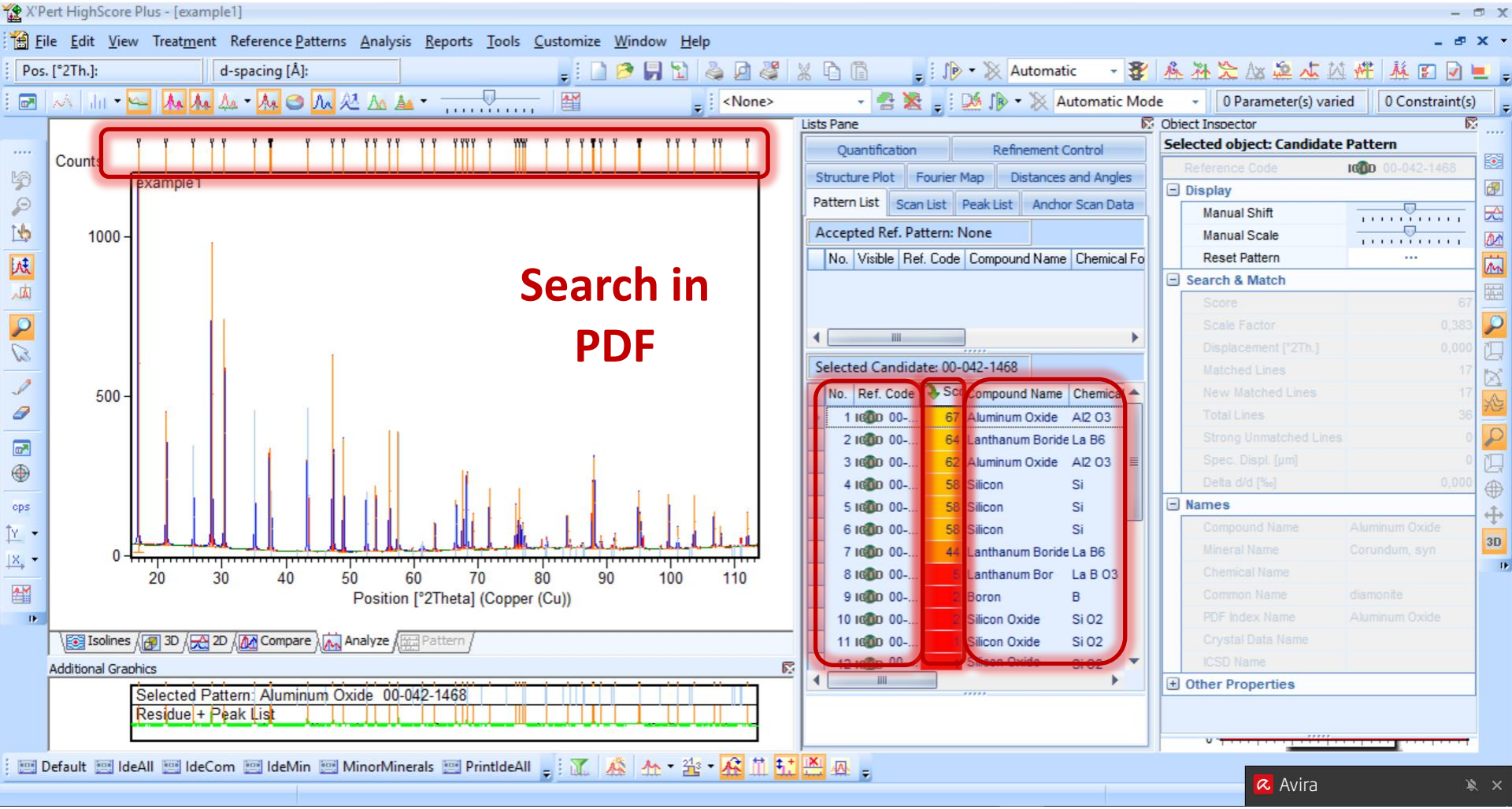

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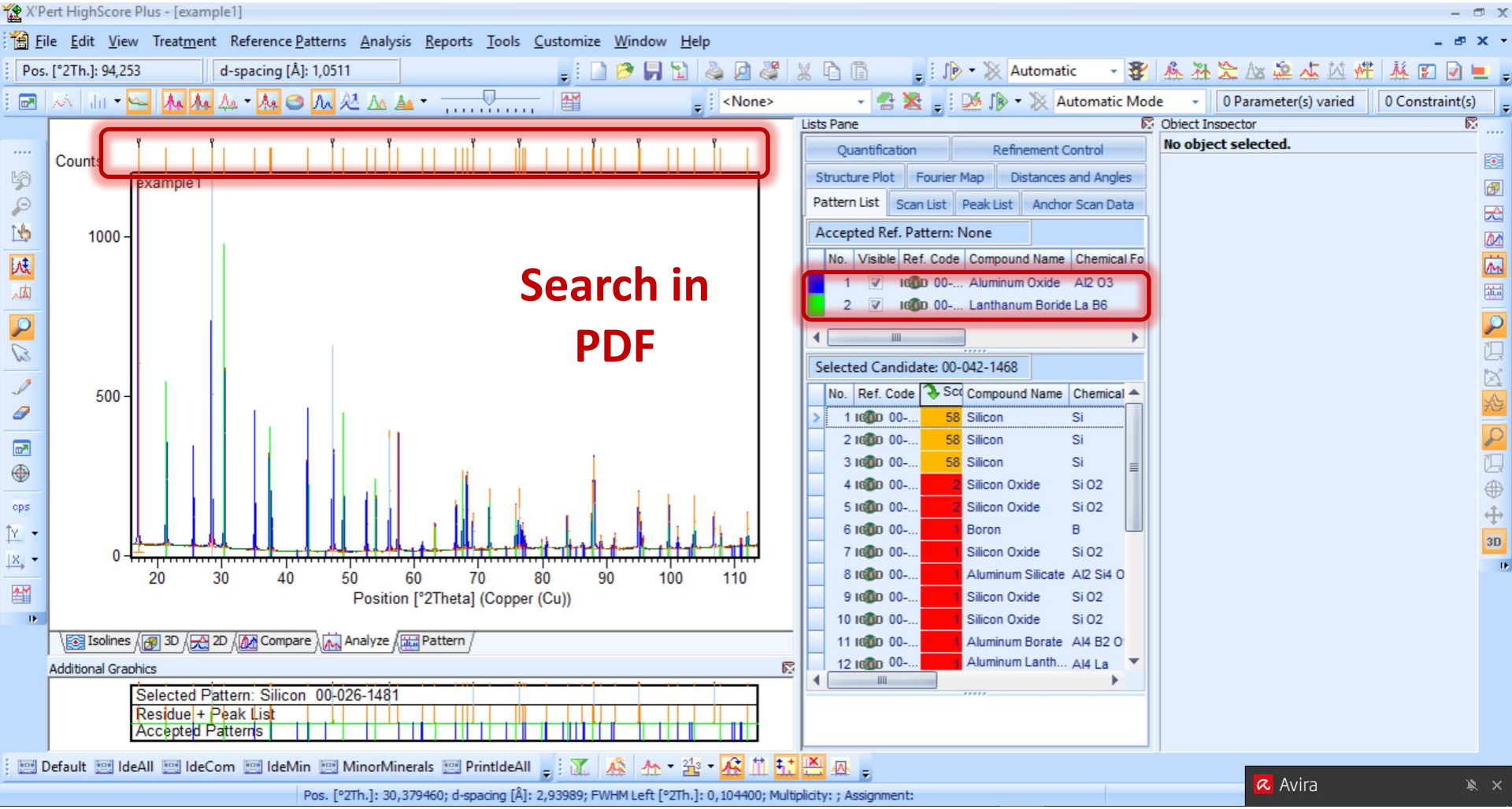

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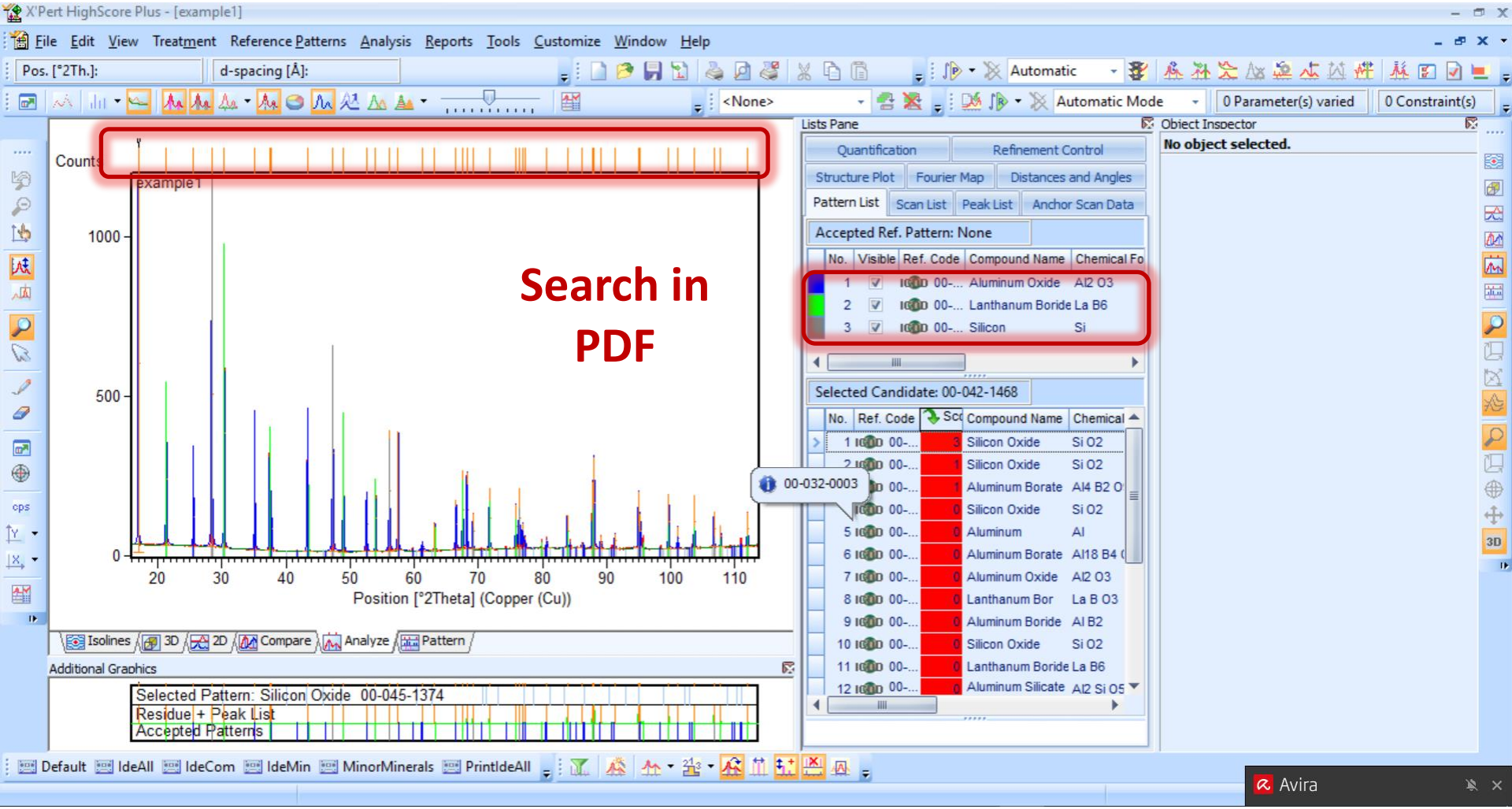

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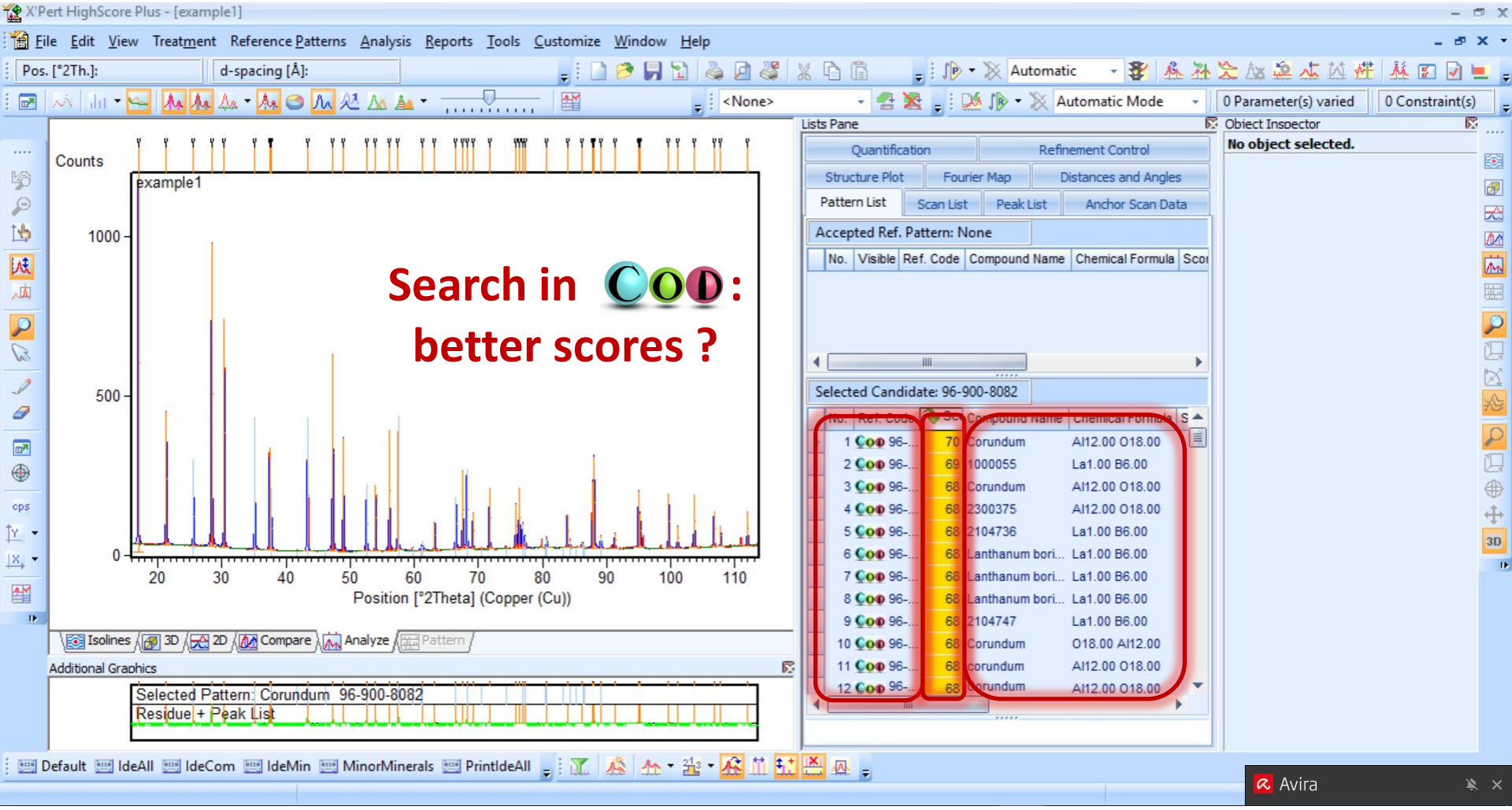
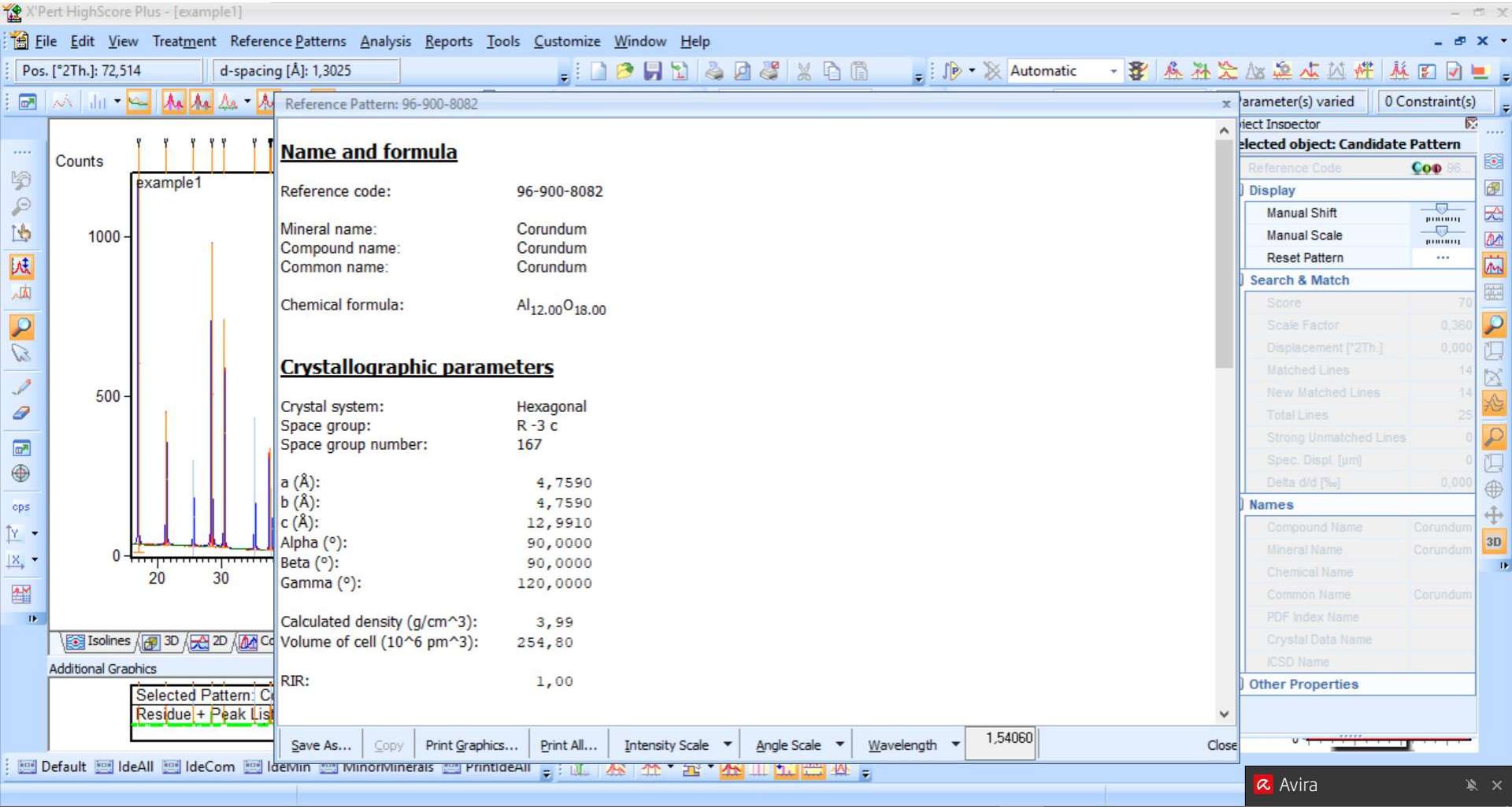
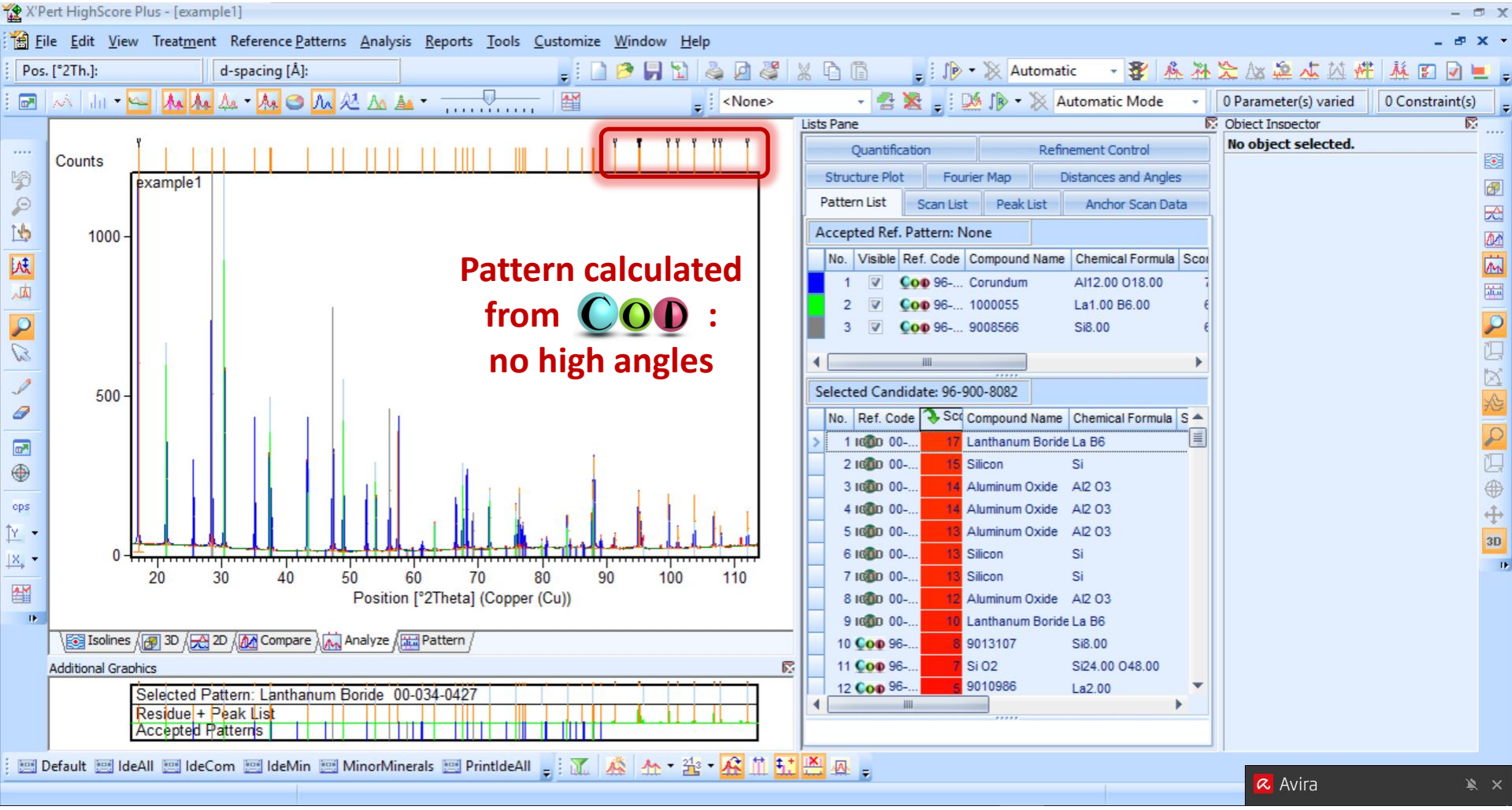


Phase identification using COD with HighScore(Plus)

COD reference patterns are accessibles as well as PDF ones

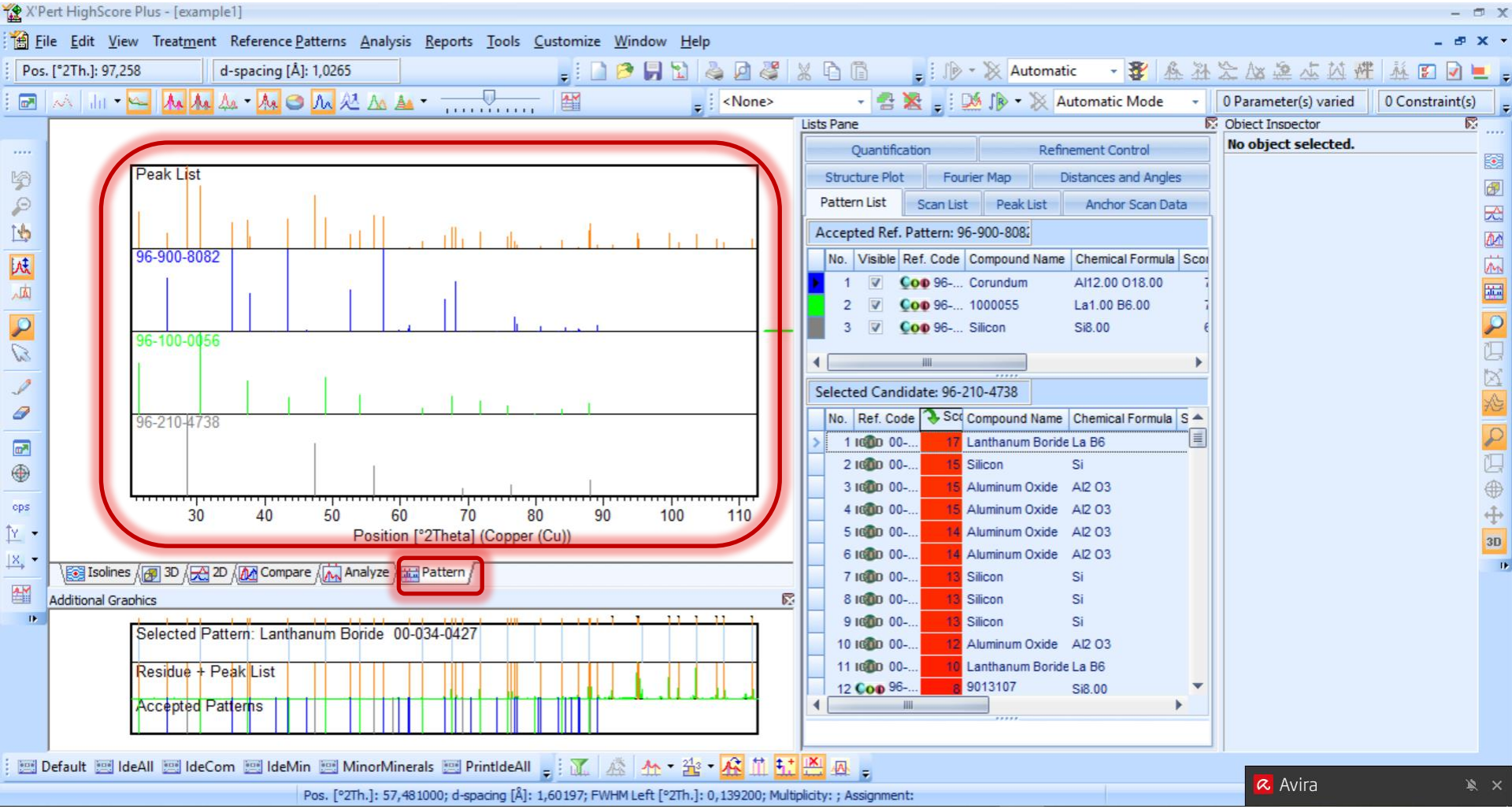


Phase identification using COD with HighScore(Plus)



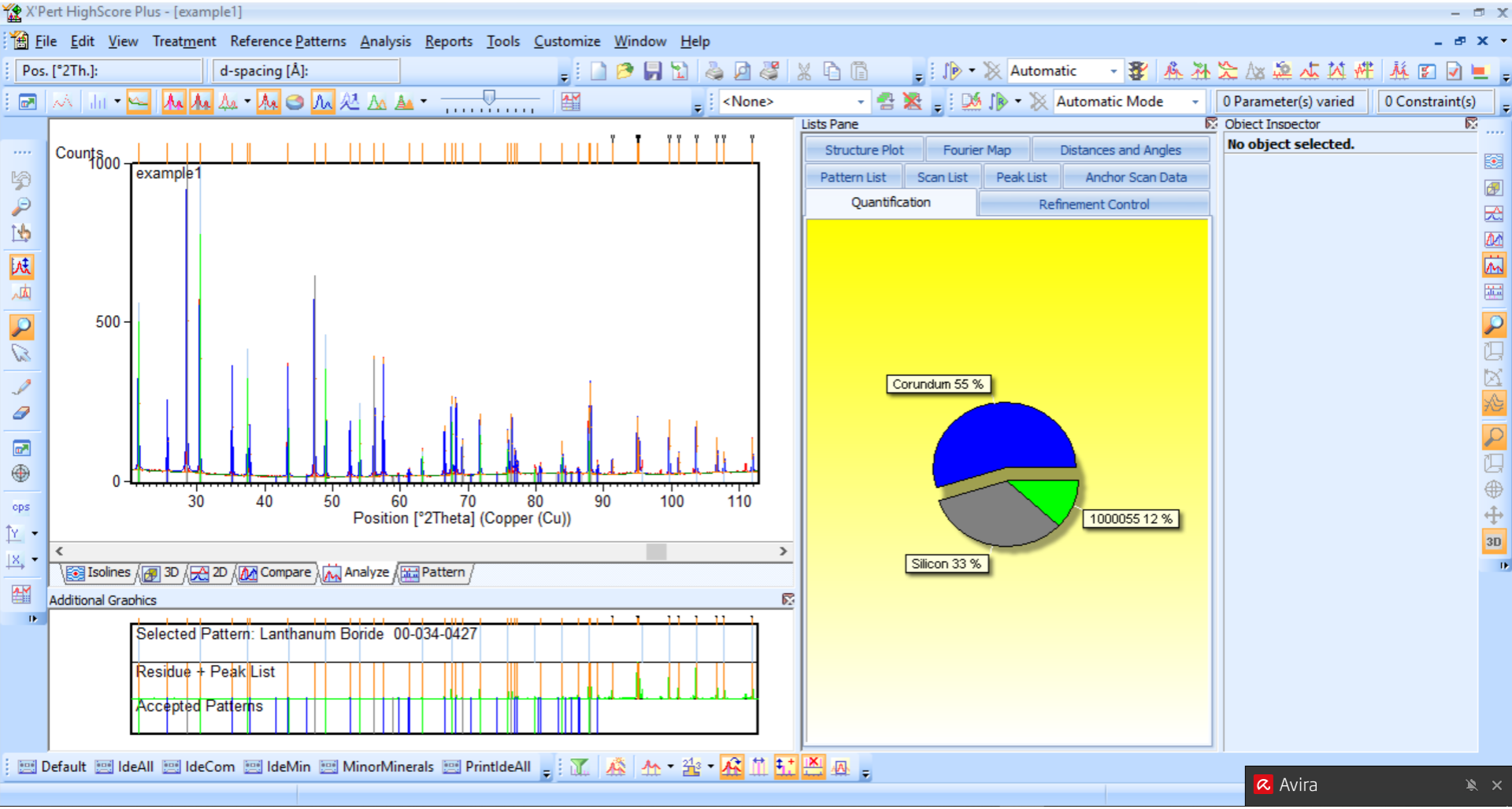
Phase identification using COD with HighScore(Plus)

Visualisation options…



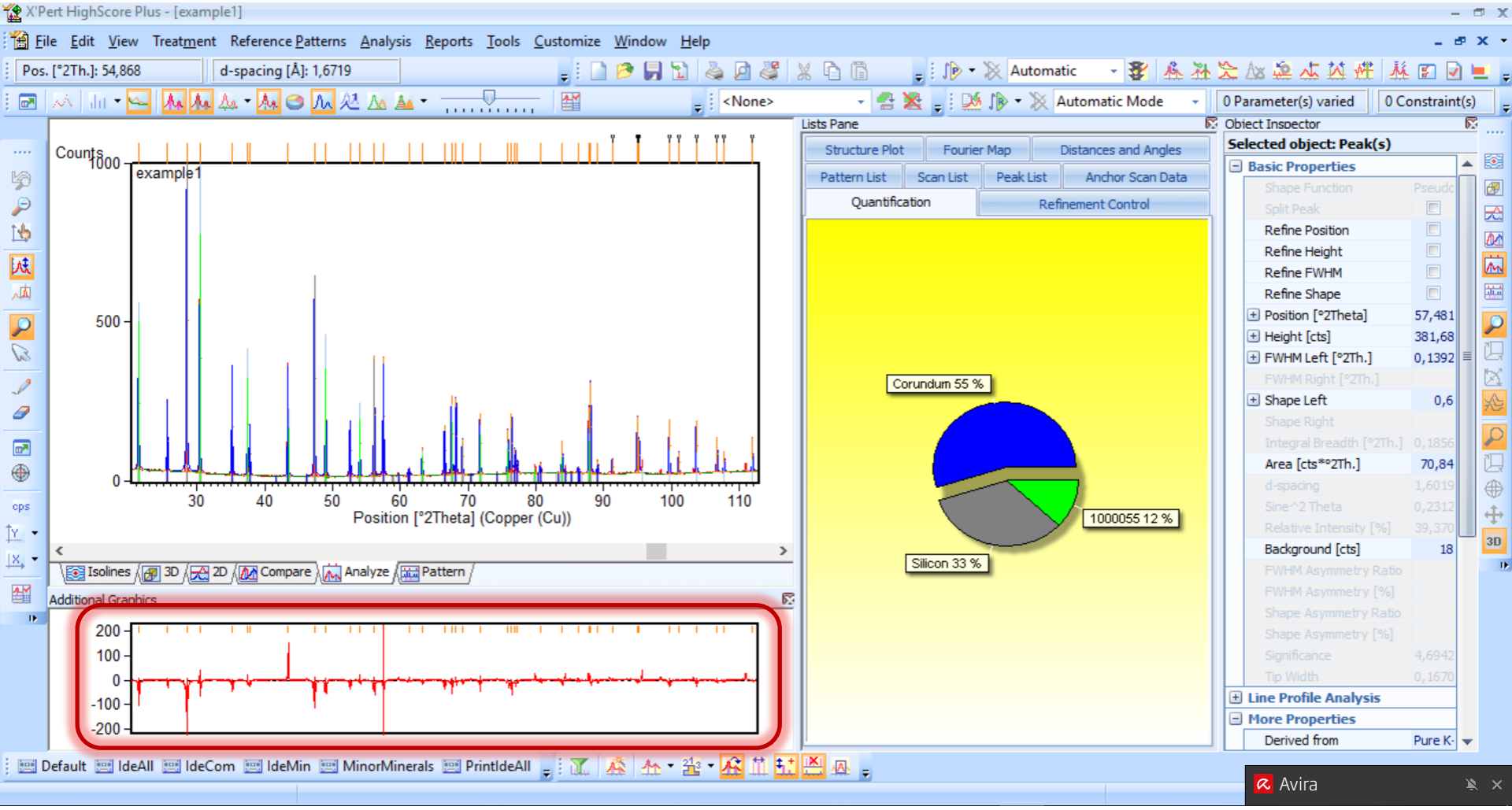
Phase identification using COD with HighScore(Plus)

« semi quantitative » analysis from RIR



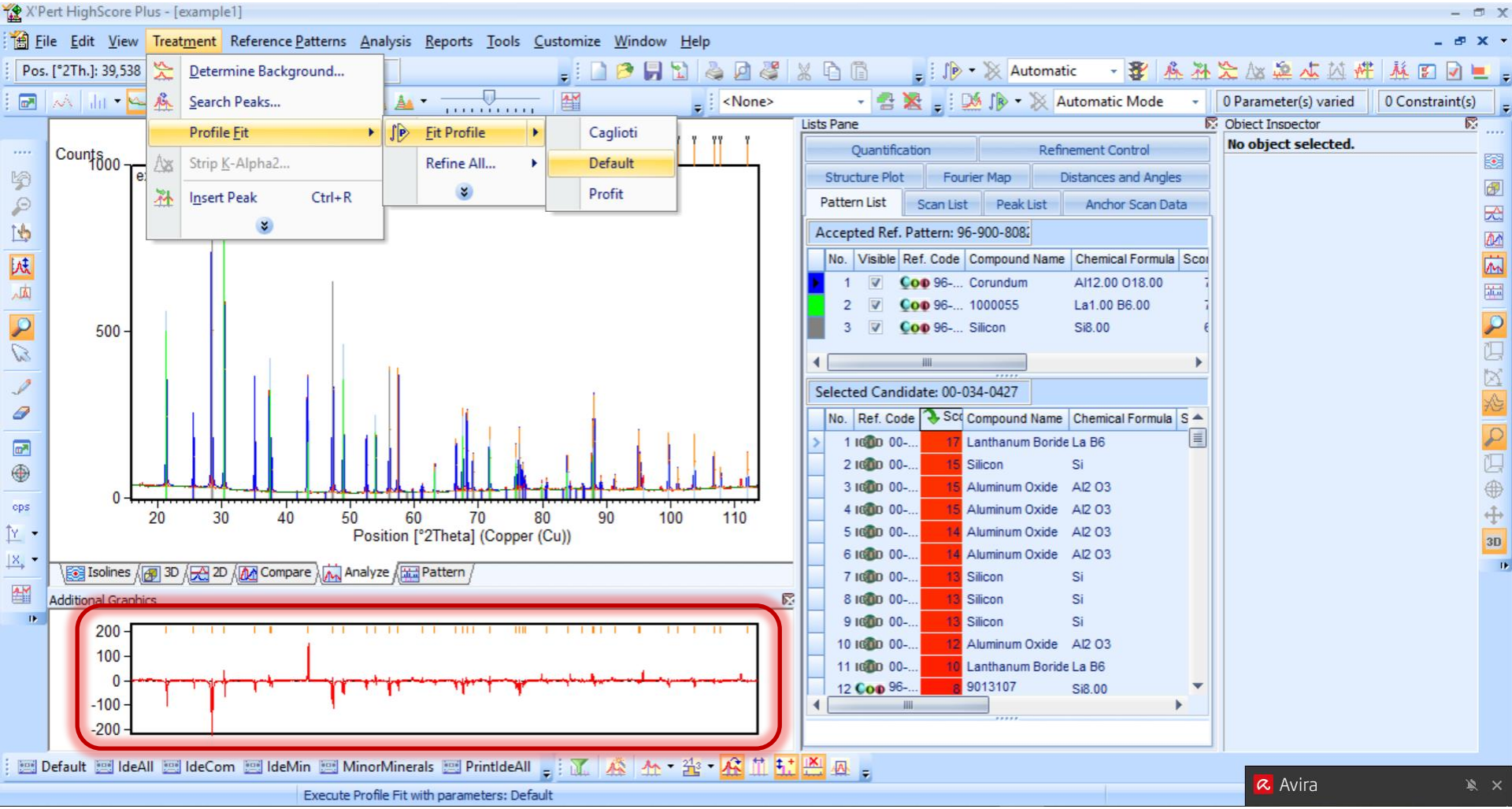
Phase identification using COD with HighScore(Plus)

« semi quantitative » analysis from RIR without refinement



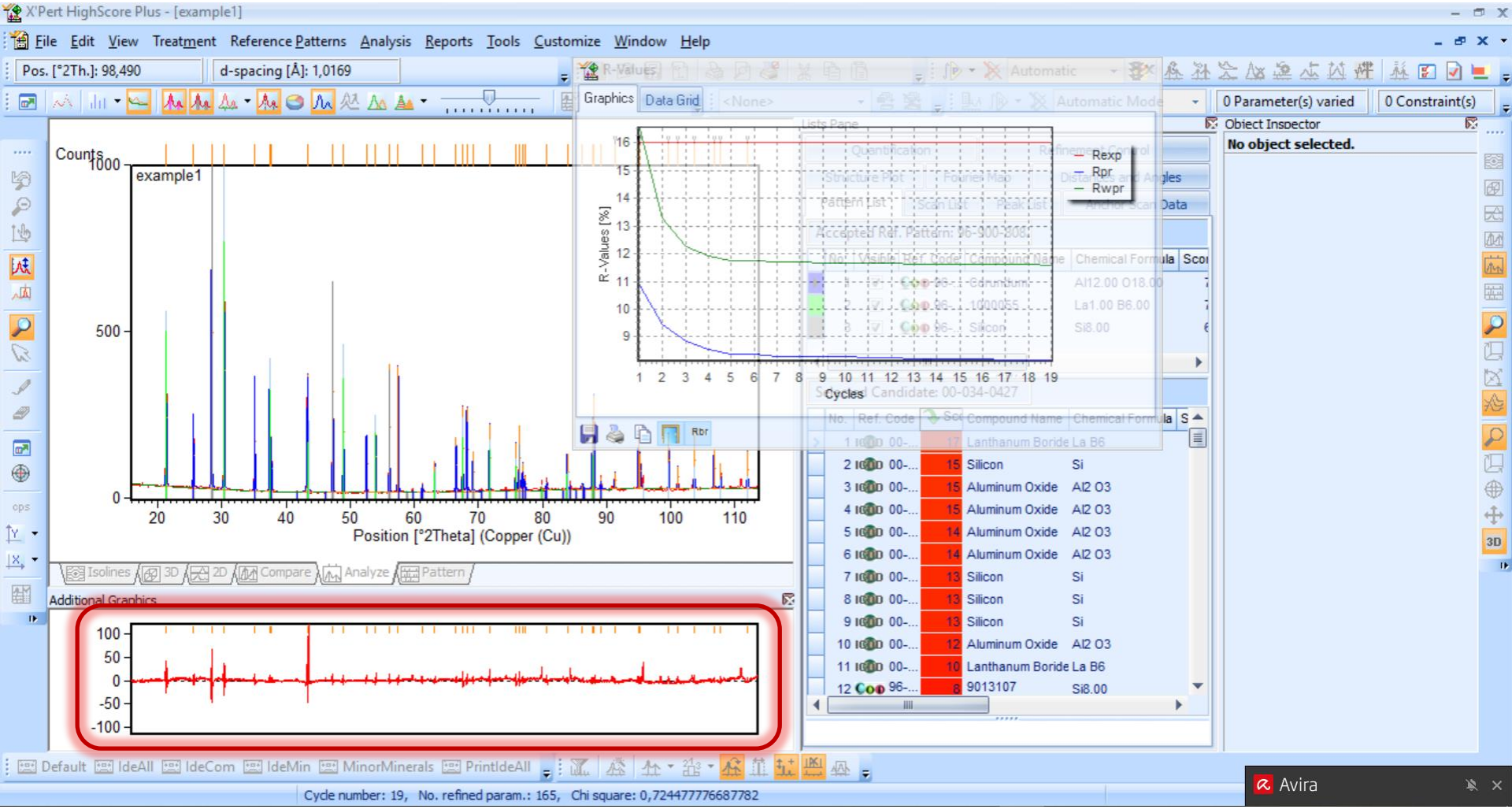
Phase identification using COD with HighScore(Plus)

« semi quantitative » analysis from RIR with an automatic profile refinement



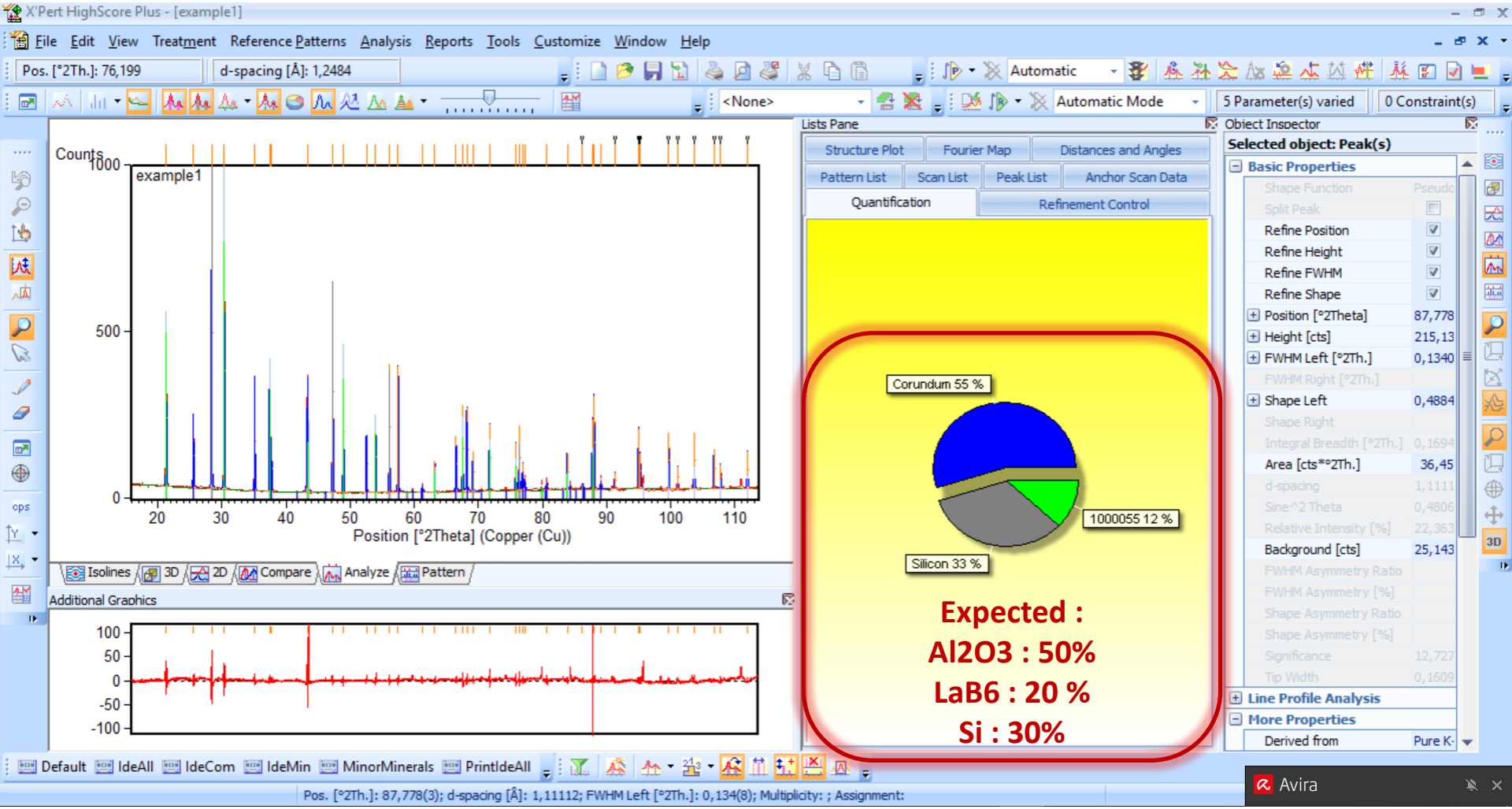
Phase identification using COD with HighScore(Plus)

« semi quantitative » analysis from RIR with an automatic profile refinement



Phase identification using COD with HighScore(Plus)

« semi quantitative » analysis from RIR with an automatic profile refinement



Phase identification using COD with QualX

Software Ic

Institute of Crystallography – CNR – Bari

Contact IC CNR

Software Available

The software packages currently developed at IC are:

- Sir: a widely used package for the solution and refinement of small single-crystal structures using either X-ray or electron diffraction data. It is also included in IL MILIONE.
- IL MILIONE: a suite of computer programs devoted to protein crystal structure determination by X-ray crystallography. The package currently contains the program *Sir2014* for the solution and refinement of small structures.
- EXPO2014: an integrated package for the indexation of a powder diffraction pattern, the extraction of integrated intensities, the space group determination, the crystal structure solution *via* Direct Methods and/or by a direct-space approach, and the structure refinement by the Rietveld technique.
- QualX2: a computer program for phase identification using powder diffraction data.
- Quanto: a Rietveld program for quantitative phase analysis of polycrystalline mixtures from powder diffraction data.
- SunBIM: a suite of programs for the supra- and sub-molecular X-ray imaging of nano and bio materials with SAXS, WAXS, GISAXS and GIWAXS techniques

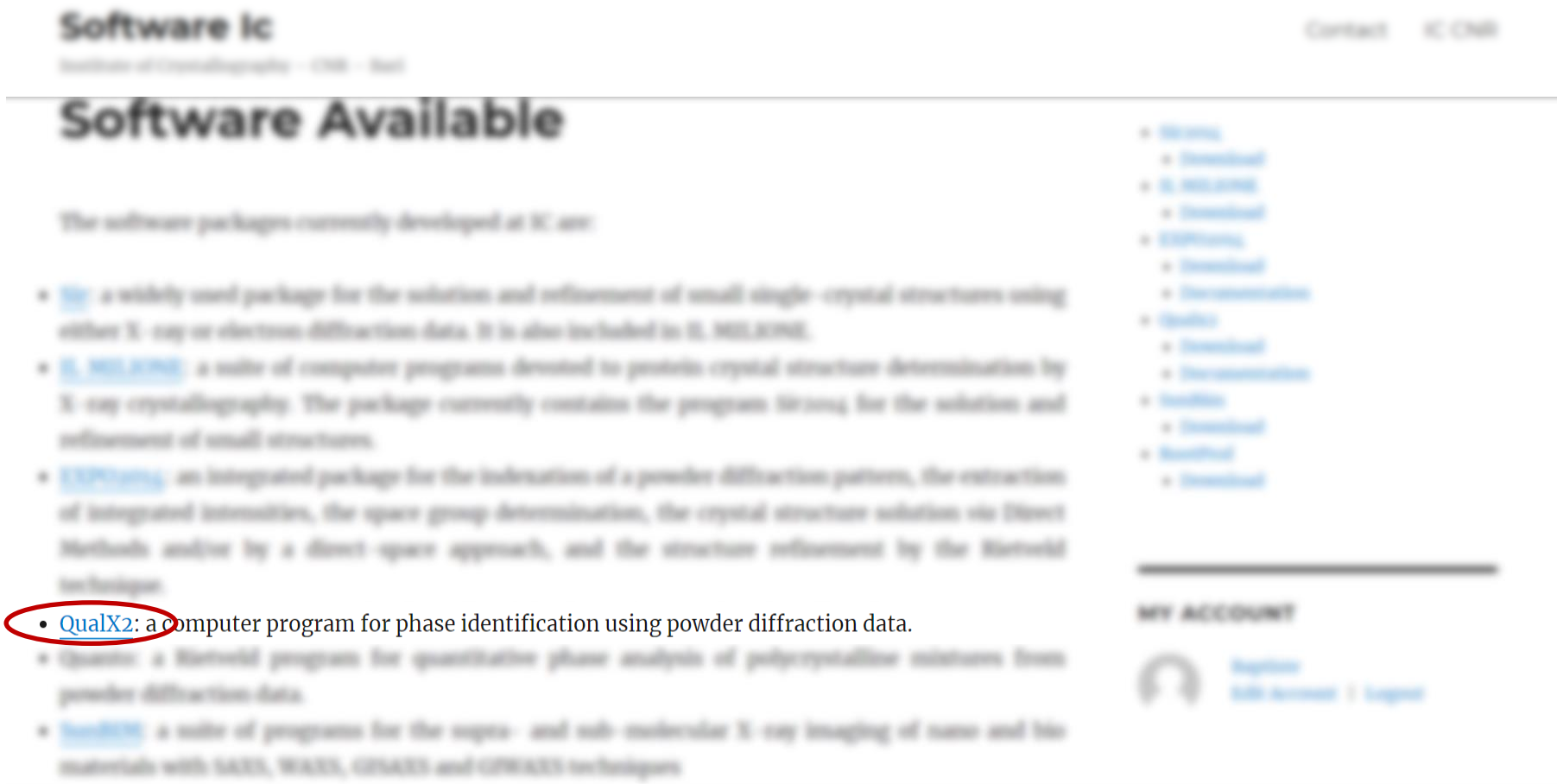
- Sir2014
  - Download
- IL MILIONE
  - Download
- EXPO2014
  - Download
  - Documentation
- Qualx2
  - Download
  - Documentation
- SunBim
  - Download
- RootProf
  - Download

MY ACCOUNT

Baptiste
Edit Account | Logout

http://www.ba.ic.cnr.it/softwareic/qualx/

Phase identification using COD with QualX



http://www.ba.ic.cnr.it/softwareic/qualx/

Phase identification using COD with QualX

QualX2 download

You are required to login to view this page.

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in QualX format →

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Powcod Download

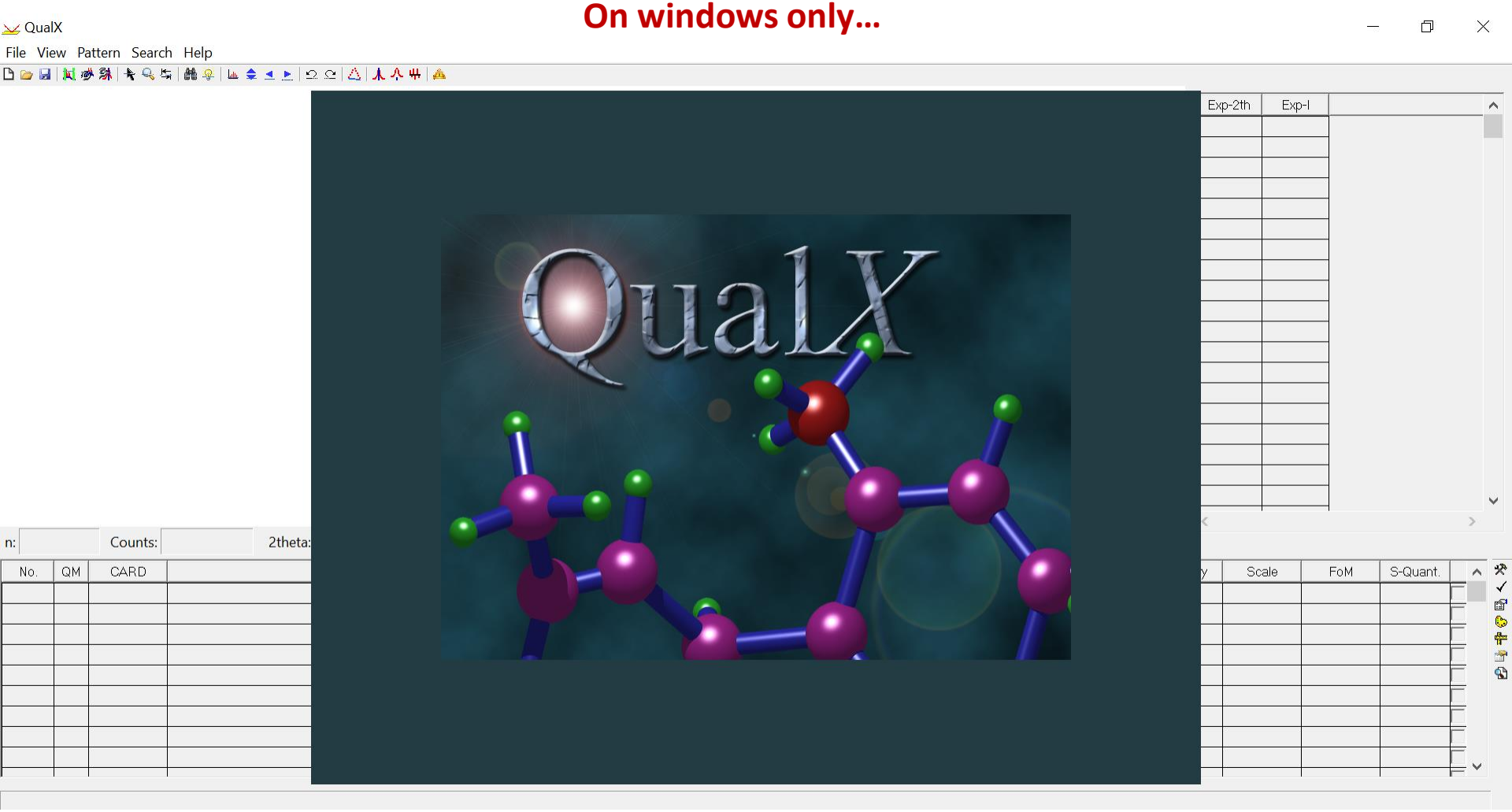
Qualx2 Download

- QualX2: a computer program for phase identification using powder diffraction data.

http://www.ba.ic.cnr.it/softwareic/qualx/

Phase identification using COD with QualX

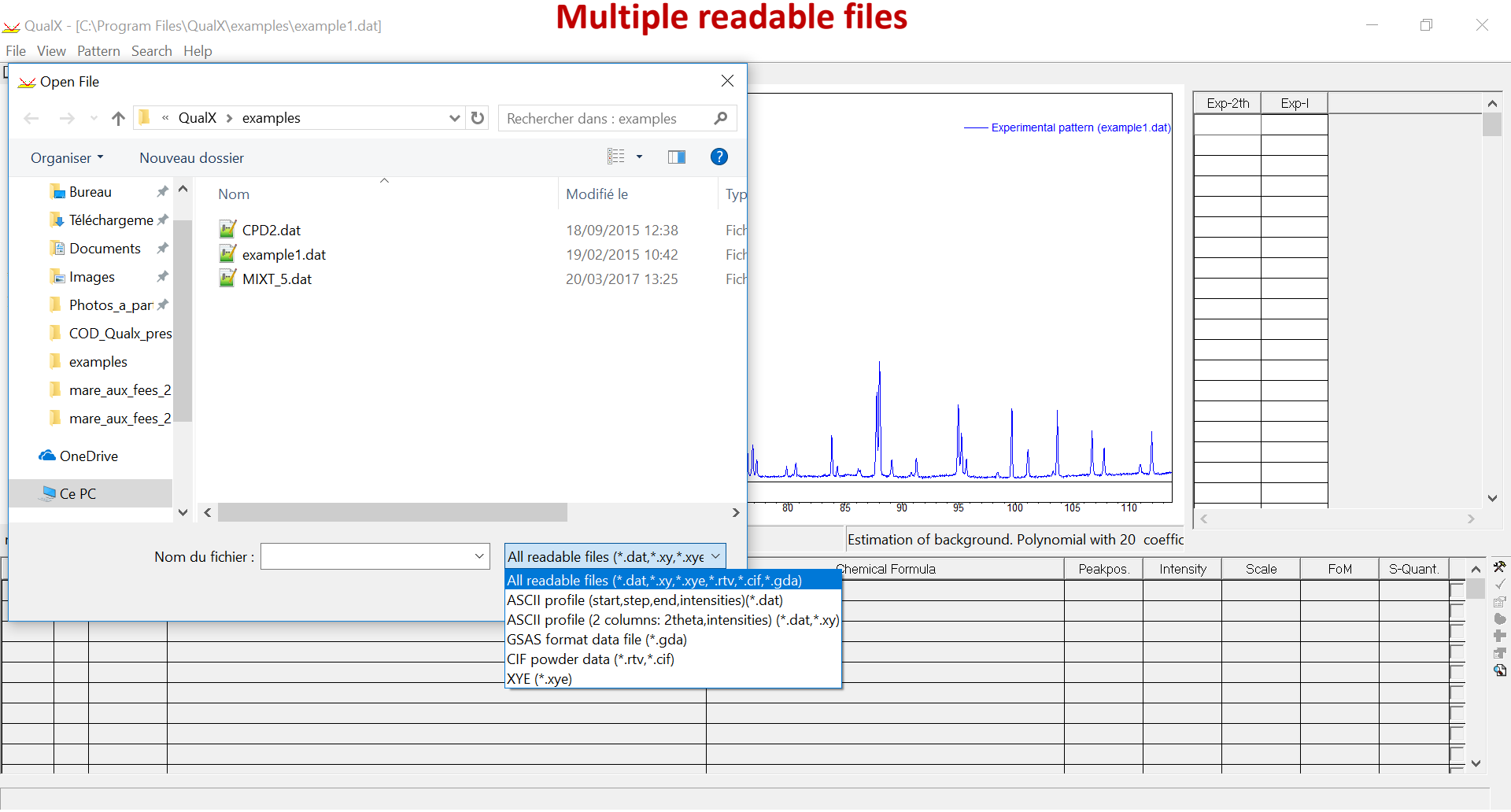
On windows only…



Altomare, A., Corriero, N., Cuocci, C., Falcicchio, A., Moliterni, A., Rizzi, R.
QUALX2.0: a qualitative phase analysis software using the freely available database POW_COD,
J. Appl. Cryst. (2015). **48**, 598-603.

Phase identification using COD with QualX

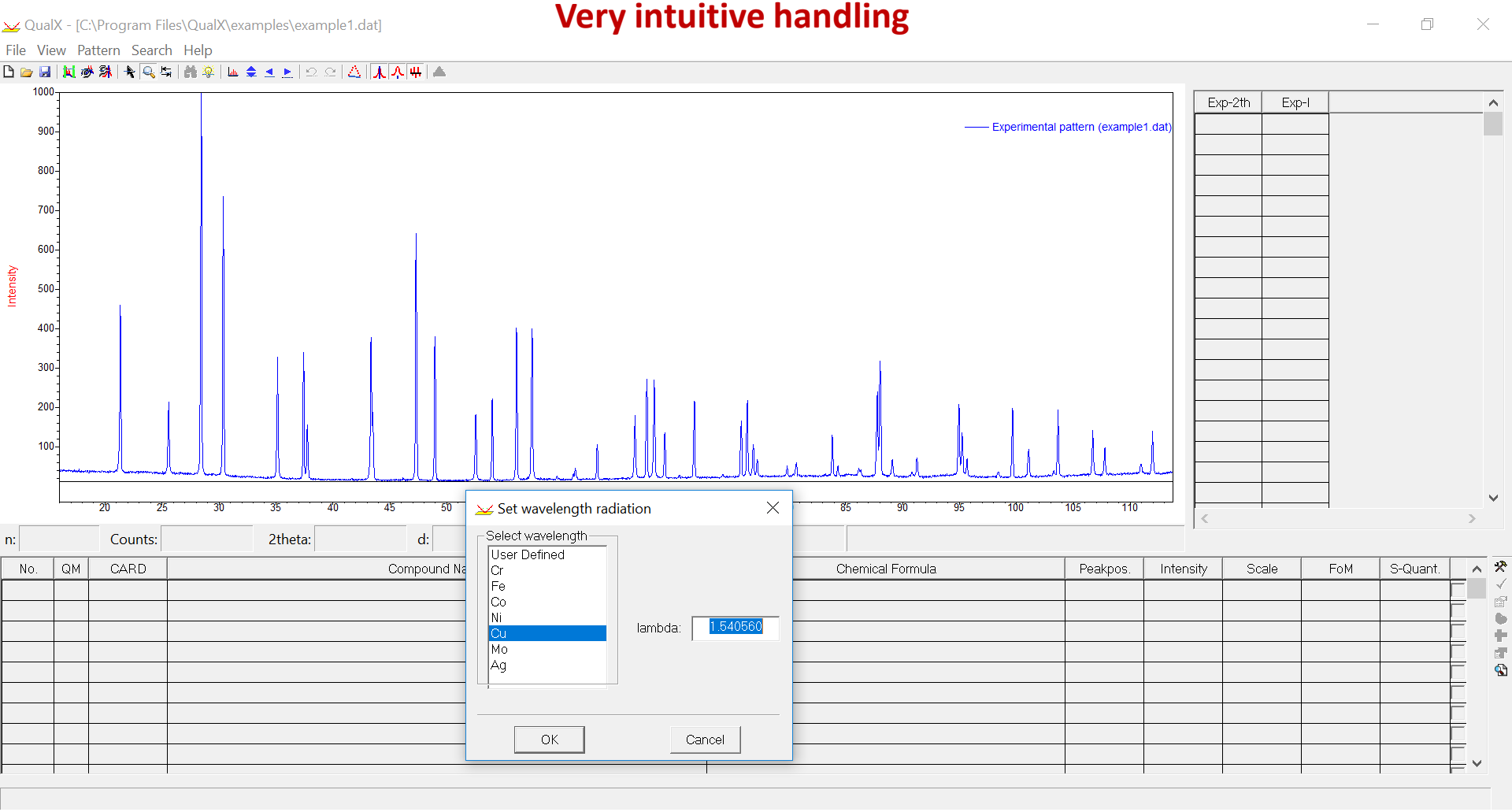
Multiple readable files



http://www.ba.ic.cnr.it/softwareic/qualx/

Phase identification using COD with QualX

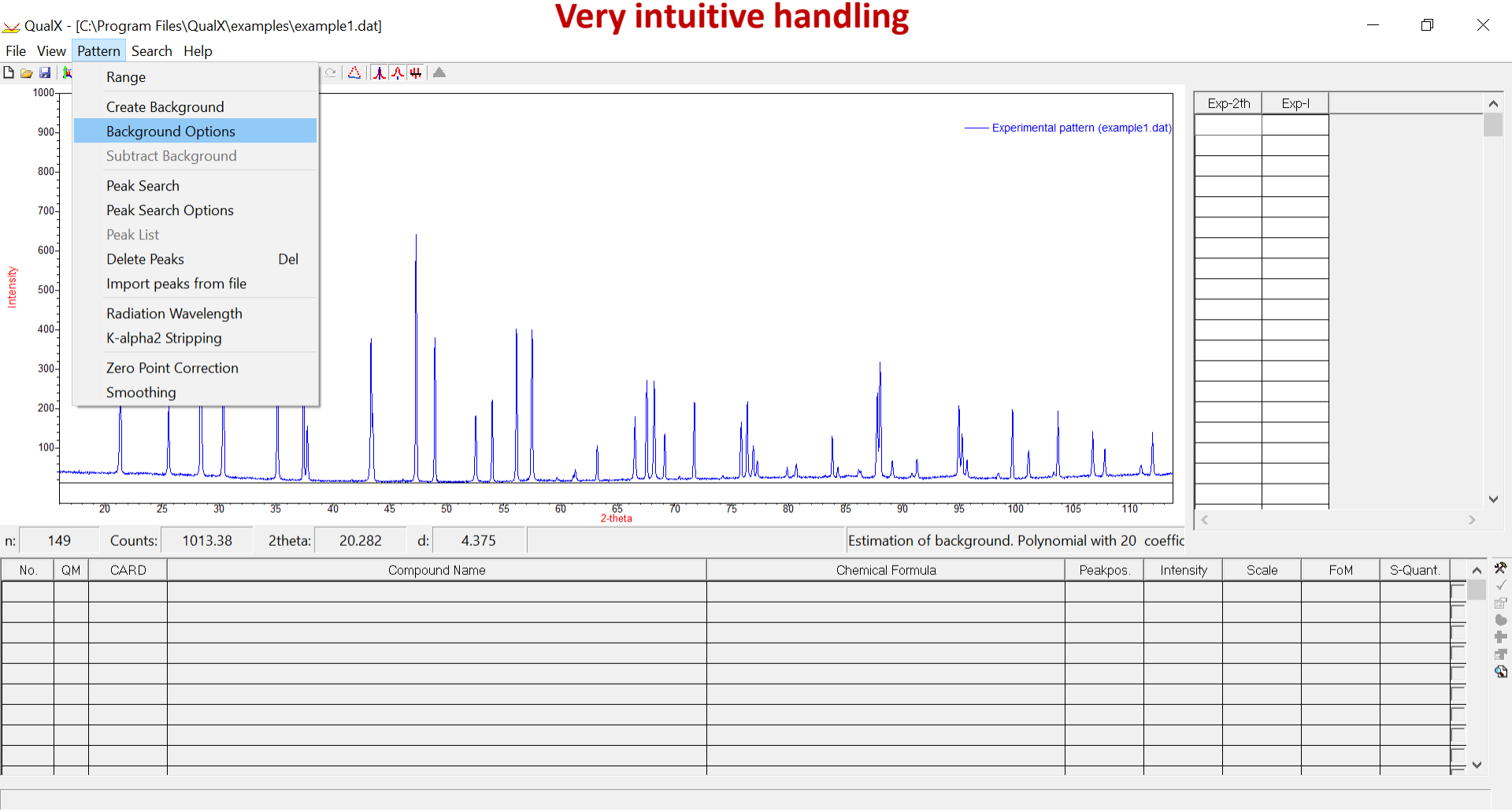
Very intuitive handling



http://www.ba.ic.cnr.it/softwareic/qualx/

Phase identification using COD with QualX

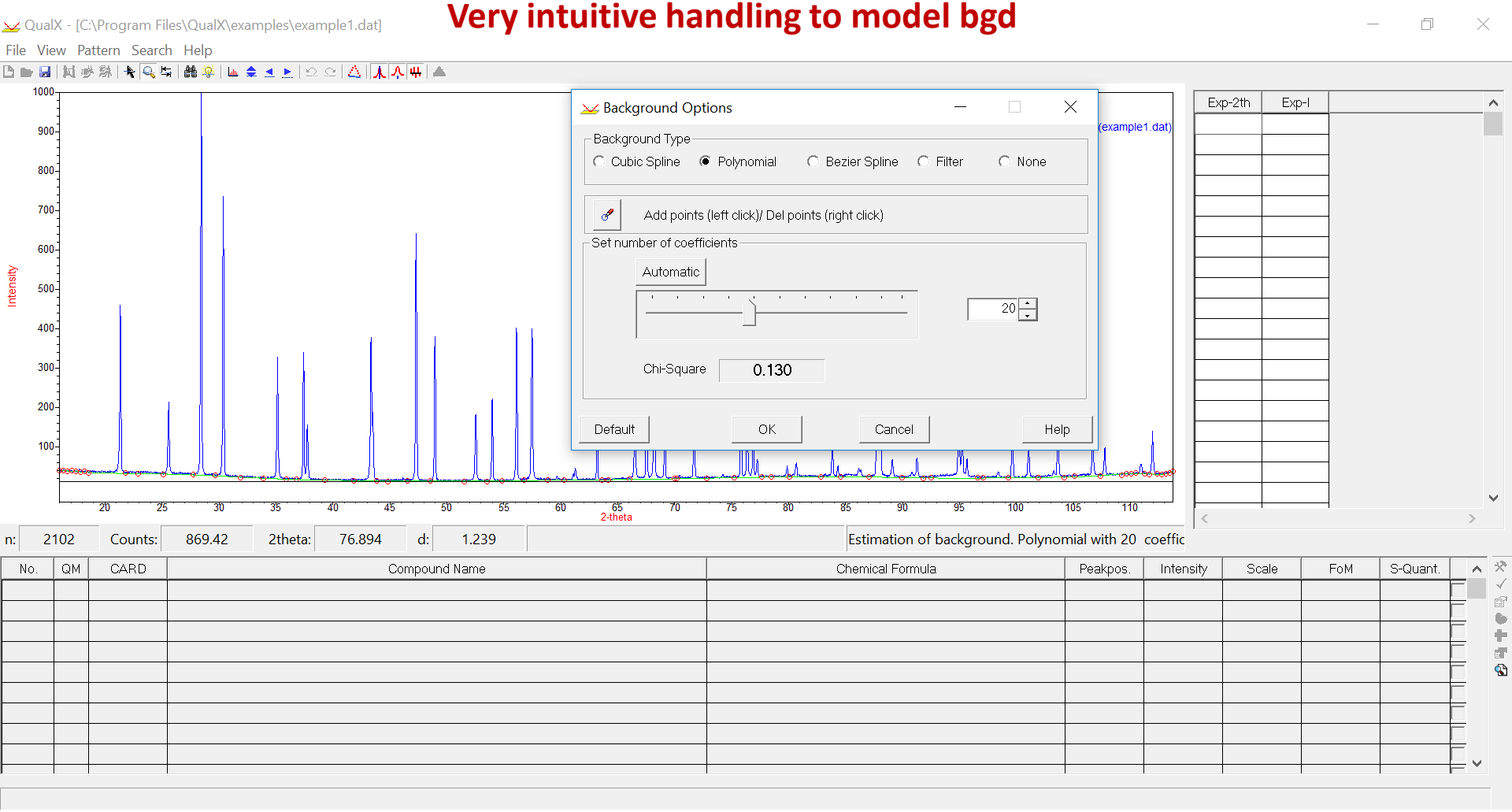
Very intuitive handling



http://www.ba.ic.cnr.it/softwareic/qualx/

Phase identification using COD with QualX

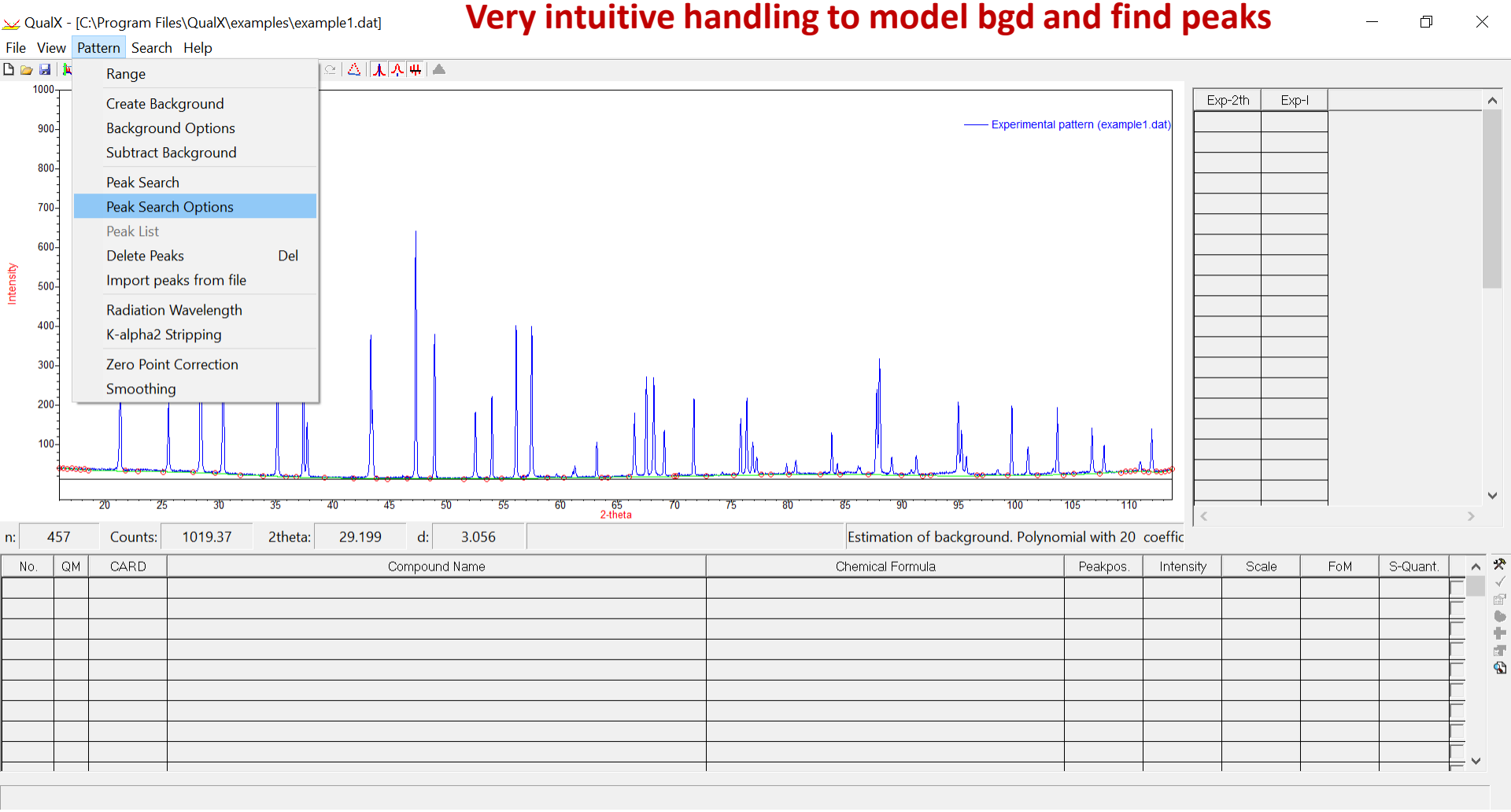
Very intuitive handling to model bgd



http://www.ba.ic.cnr.it/softwareic/qualx/

Phase identification using COD with QualX

Very intuitive handling to model bgd and find peaks



http://www.ba.ic.cnr.it/softwareic/qualx/

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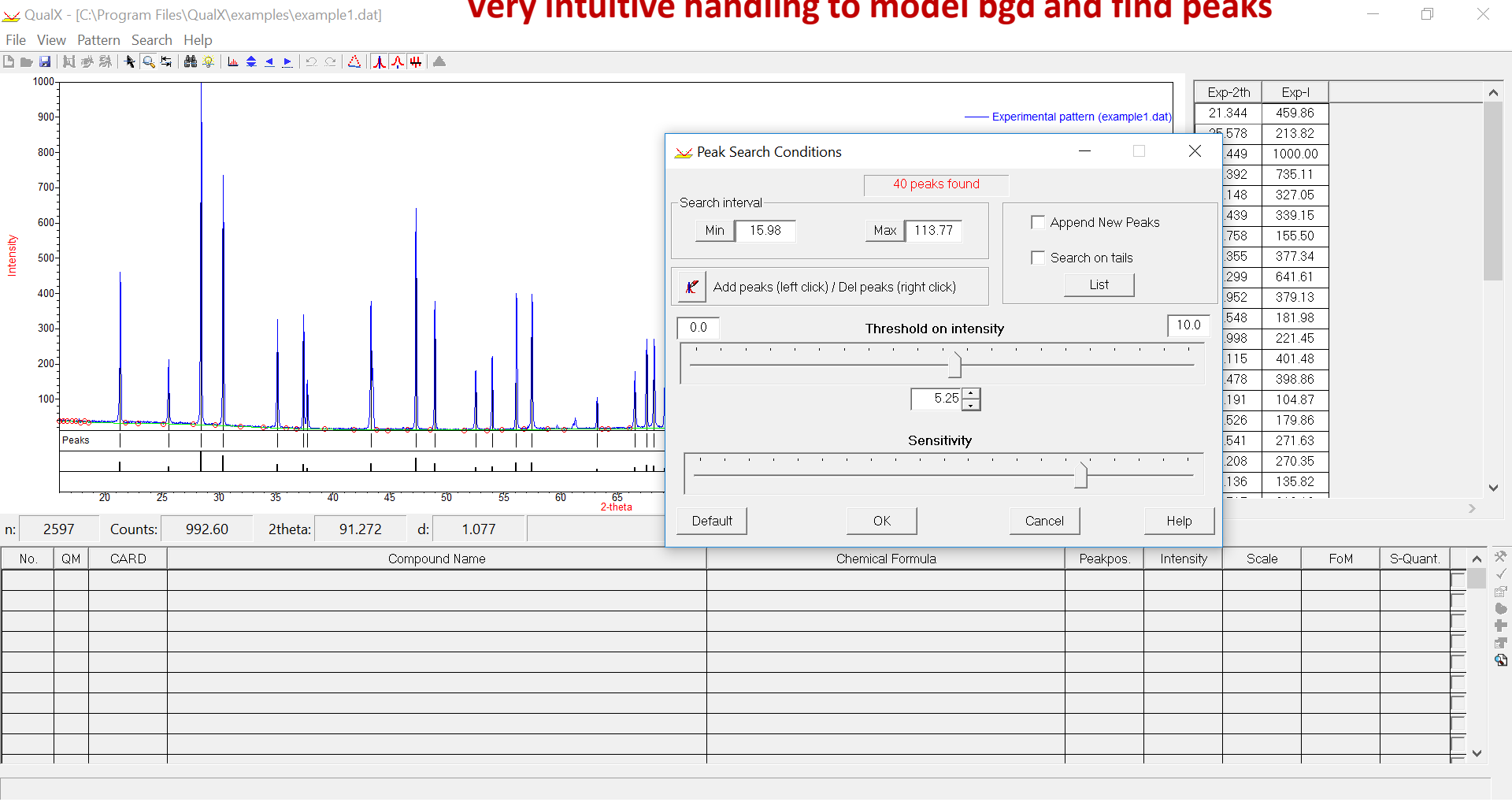
Very intuitive handling to model bgd and find peaks



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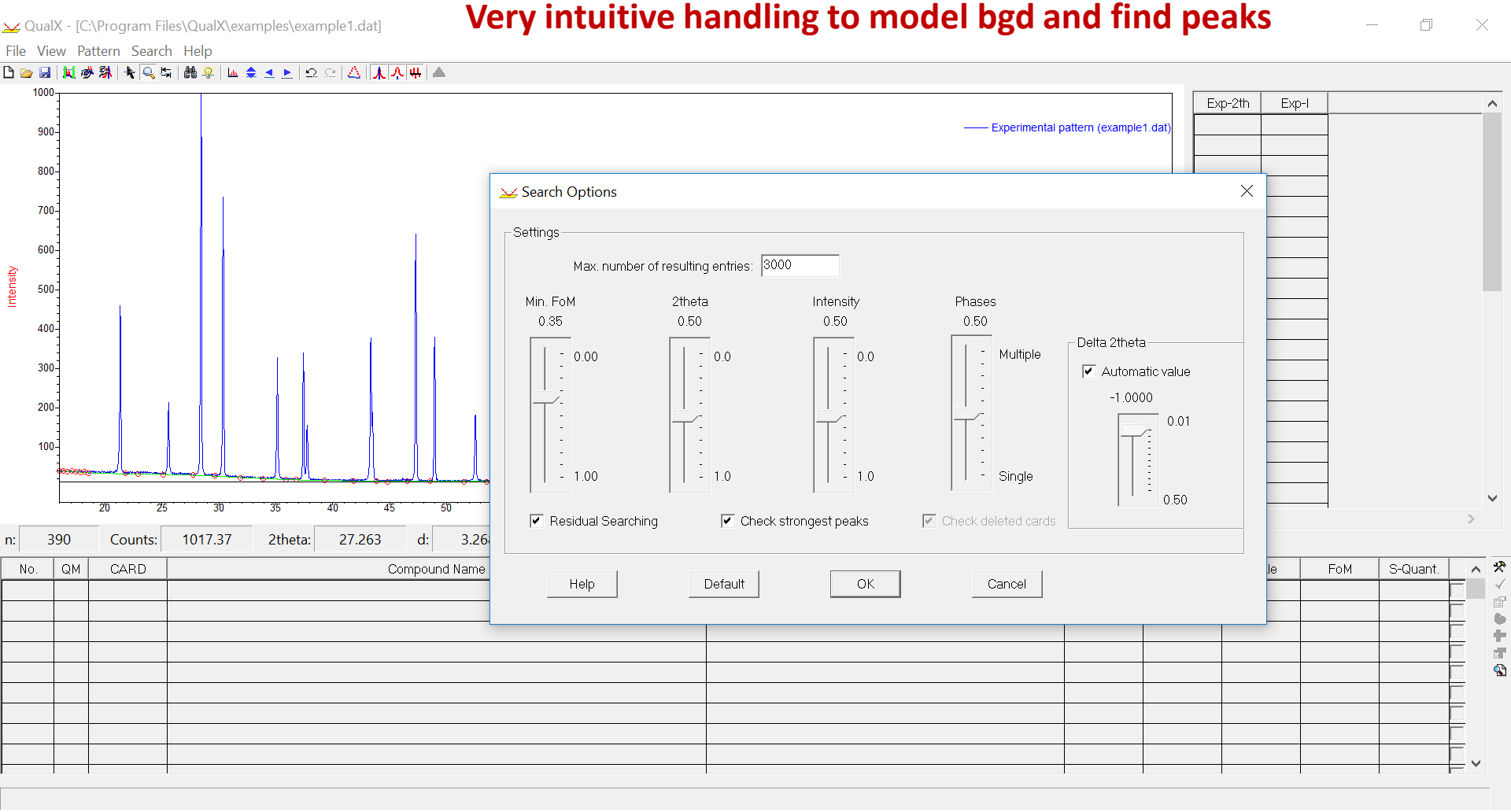
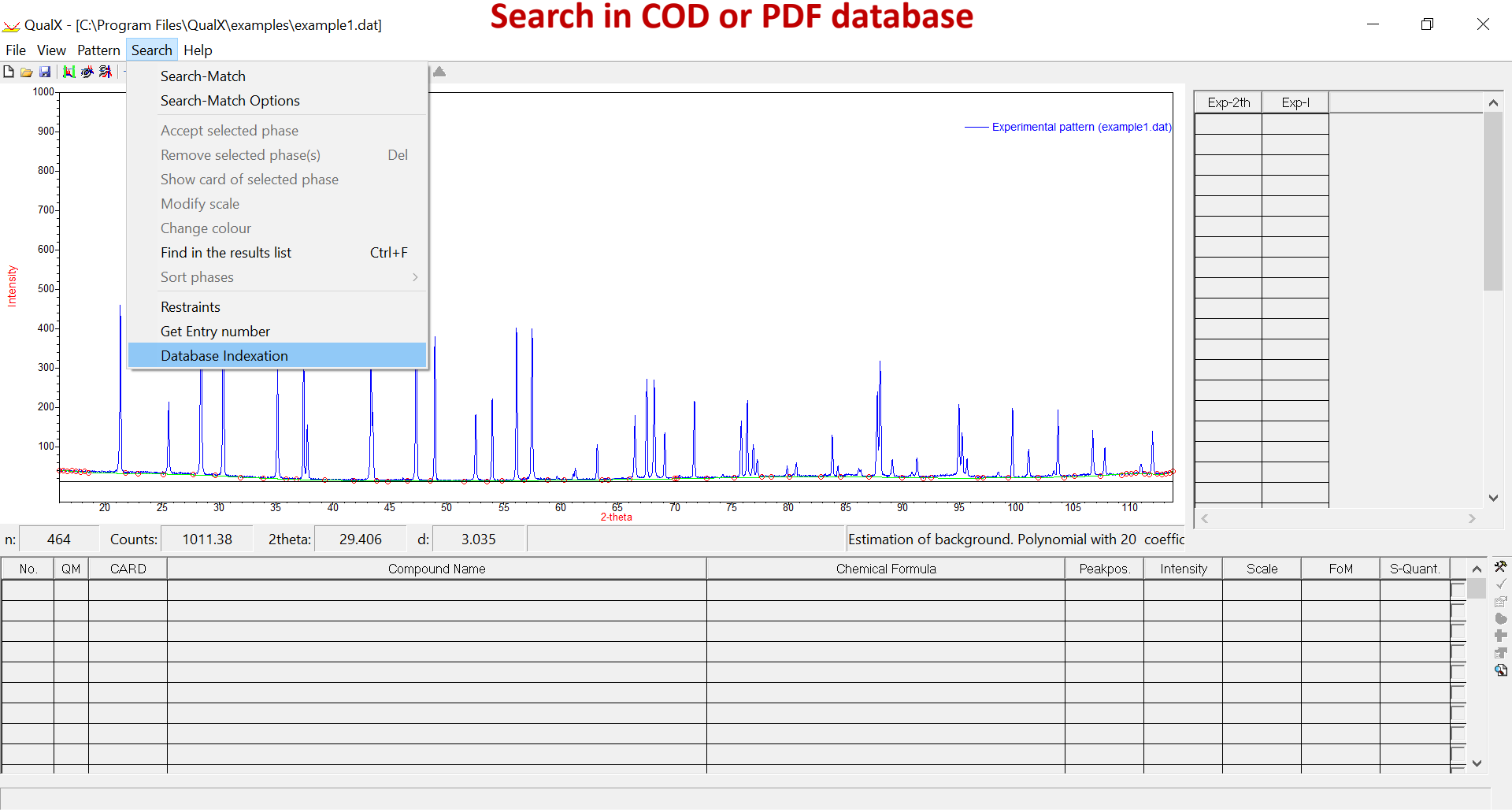


http://www.ba.ic.cnr.it/softwareic/qualx/

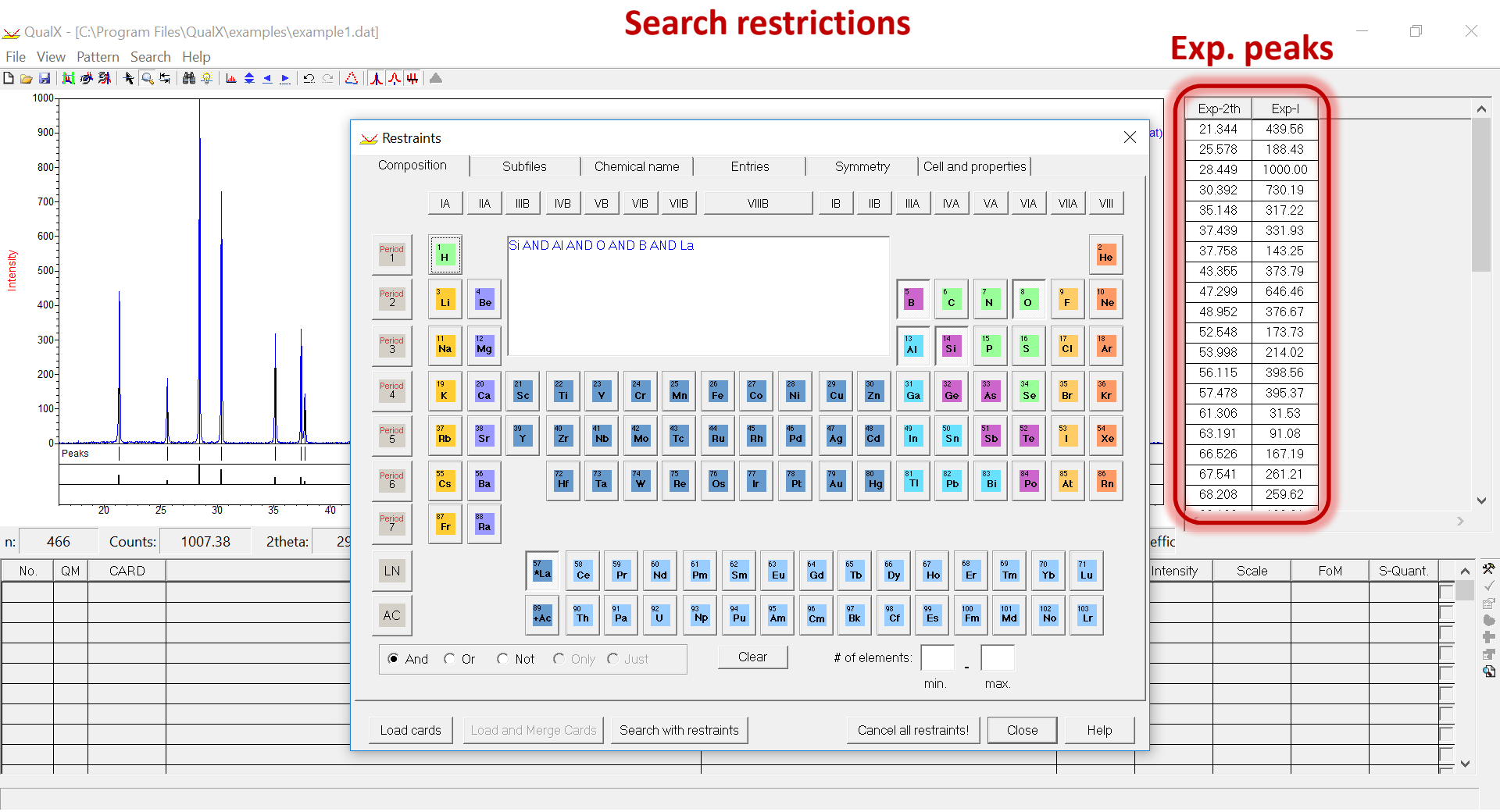
Phase identification using COD with QualX

Search in COD or PDF database



http://www.ba.ic.cnr.it/softwareic/qualx/

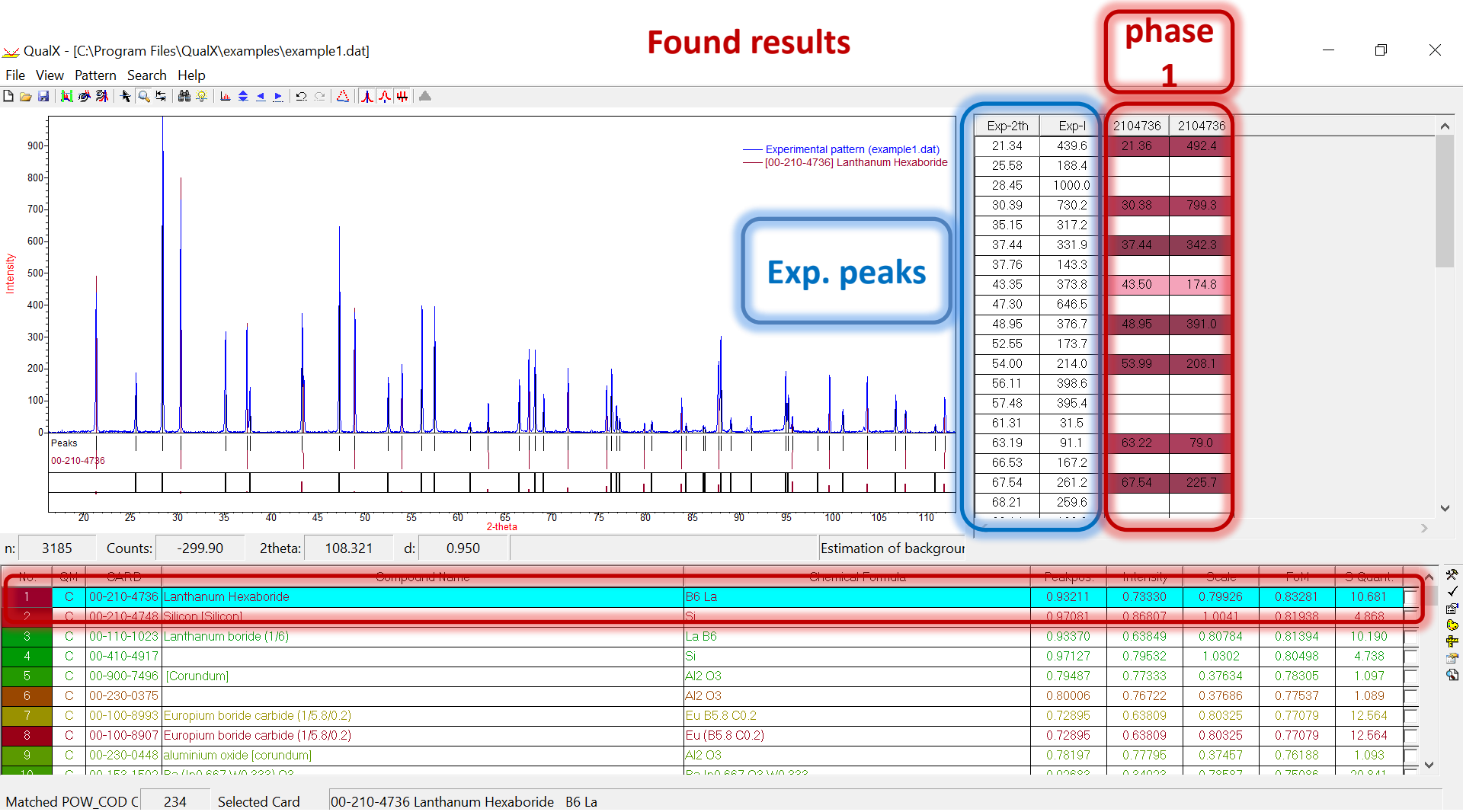
Phase identification using COD with QualX



http://www.ba.ic.cnr.it/softwareic/qualx/

Phase identification using COD with QualX

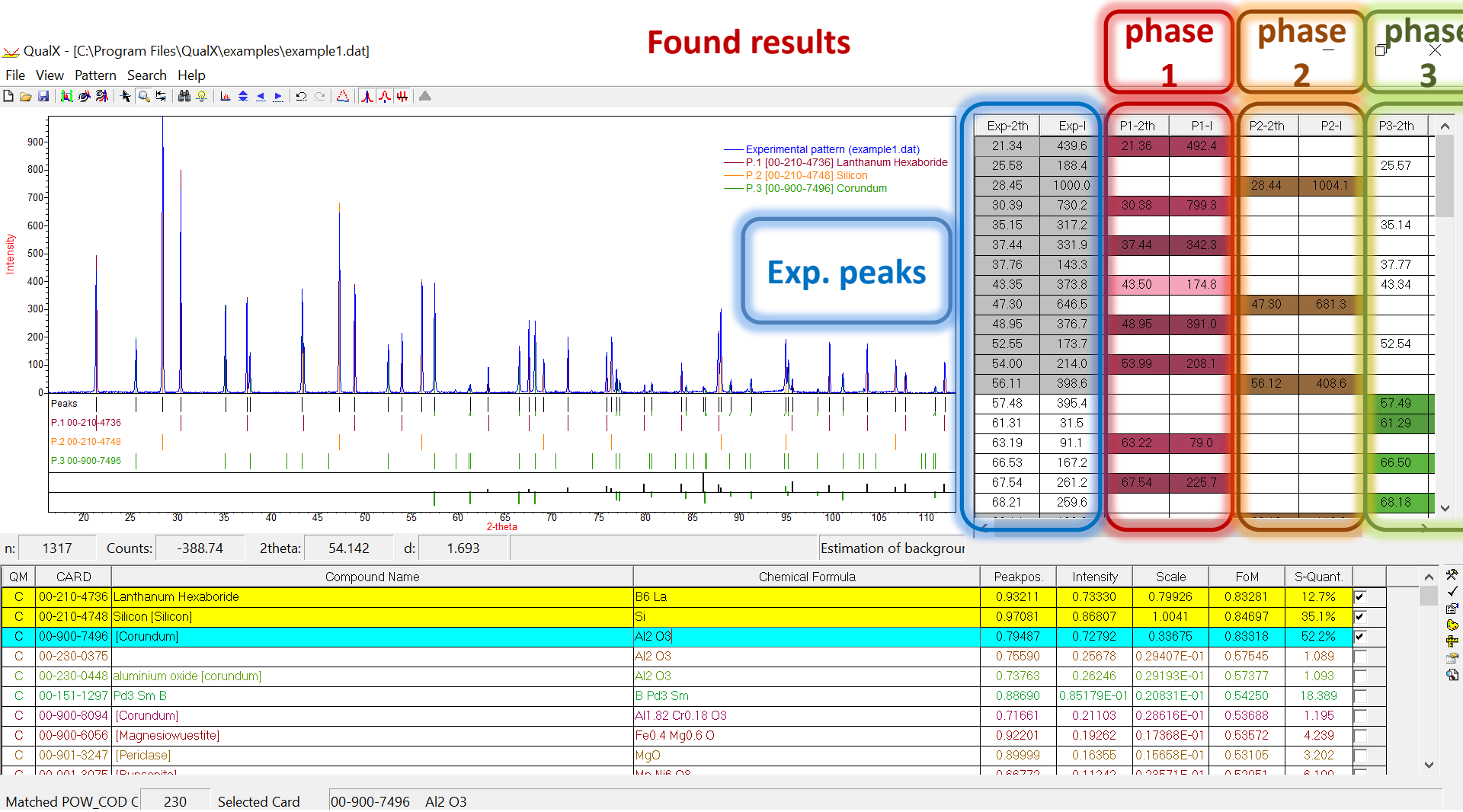
Found results



http://www.ba.ic.cnr.it/softwareic/qualx/

Phase identification using COD with QualX

Found results



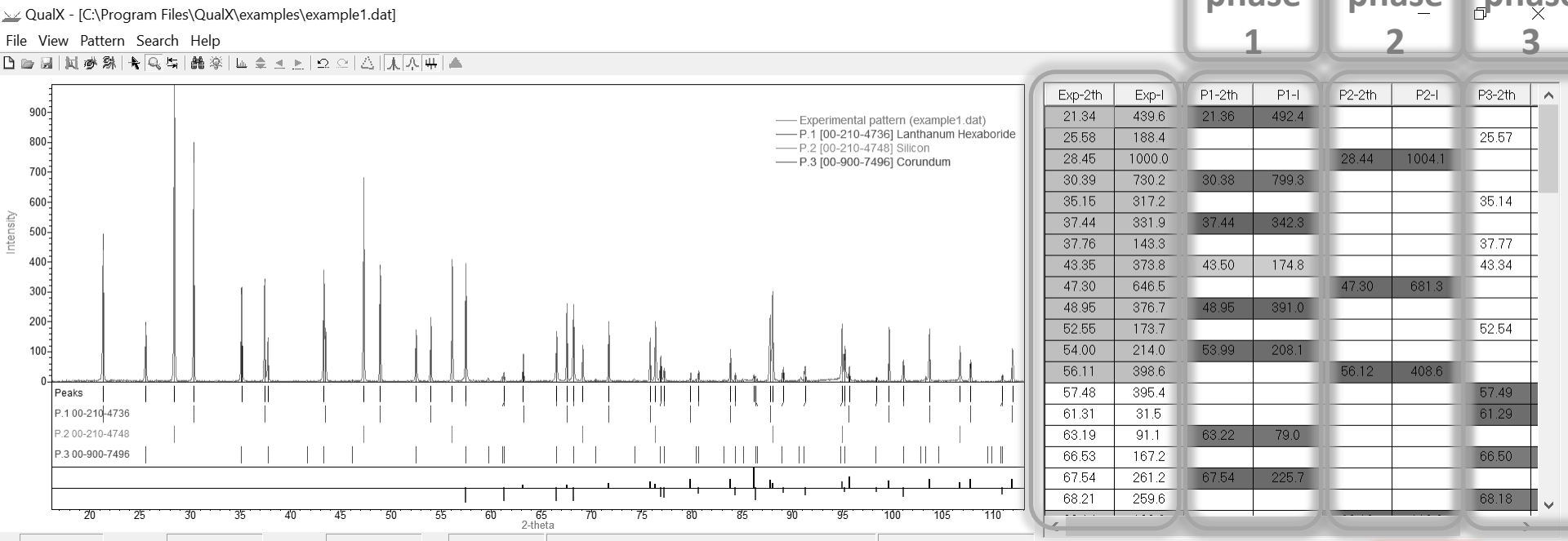
Exp-2th	Exp-I	P1-2th	P1-I	P2-2th	P2-I	P3-2th
21.34	439.6	21.36	492.4			
25.58	188.4					25.57
28.45	1000.0			28.44	1004.1	
30.39	730.2	30.38	799.3			
35.15	317.2					35.14
37.44	331.9	37.44	342.3			
37.76	143.3					37.77
43.35	373.8	43.50	174.8			43.34
47.30	646.5			47.30	681.3	
48.95	376.7	48.95	391.0			
52.55	173.7					52.54
54.00	214.0	53.99	208.1			
56.11	398.6			56.12	408.6	
57.48	395.4					57.49
61.31	31.5					61.29
63.19	91.1	63.22	79.0			
66.53	167.2					66.50
67.54	261.2	67.54	225.7			
68.21	259.6					68.18

QM	CARD	Compound Name	Chemical Formula	Peakpos.	Intensity	Scale	FoM	S-Quant.	
C	00-210-4736	Lanthanum Hexaboride	B6 La	0.93211	0.73330	0.79926	0.83281	12.7%	☑
C	00-210-4748	Silicon [Silicon]	Si	0.97081	0.86807	1.0041	0.84697	35.1%	☑
C	00-900-7496	[Corundum]	Al2 O3	0.79487	0.72792	0.33675	0.83318	52.2%	☑
C	00-230-0375		Al2 O3	0.75590	0.25678	0.29407E-01	0.57545	1.089	☐
C	00-230-0448	aluminium oxide [corundum]	Al2 O3	0.73763	0.26246	0.29193E-01	0.57377	1.093	☐
C	00-151-1297	Pd3 Sm B	B Pd3 Sm	0.88690	0.85179E-01	0.20831E-01	0.54250	18.389	☐
C	00-900-8094	[Corundum]	Al1.82 Cr0.18 O3	0.71661	0.21103	0.28616E-01	0.53688	1.195	☐
C	00-900-6056	[Magnesiowuestite]	Fe0.4 Mg0.6 O	0.92201	0.19262	0.17368E-01	0.53572	4.239	☐
C	00-901-3247	[Periclase]	MgO	0.89999	0.16355	0.15658E-01	0.53105	3.202	☐

Matched POW_COD C 230 Selected Card 00-900-7496 Al2 O3

http://www.ba.ic.cnr.it/softwareic/qualx/

Phase identification using COD with QualX



phase 1		phase 2		phase 3
Exp-2th	Exp-I	P1-2th	P1-I	P2-2th	P2-I	P3-2th
21.34	439.6	21.36	492.4			
25.58	188.4					25.57
28.45	1000.0			28.44	1004.1	
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35.15	317.2					35.14
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37.76	143.3					37.77
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47.30	646.5			47.30	681.3	
48.95	376.7	48.95	391.0			
52.55	173.7					52.54
54.00	214.0	53.99	208.1			
56.11	398.6			56.12	408.6	
57.48	395.4					57.49
61.31	31.5					61.29
63.19	91.1	63.22	79.0			
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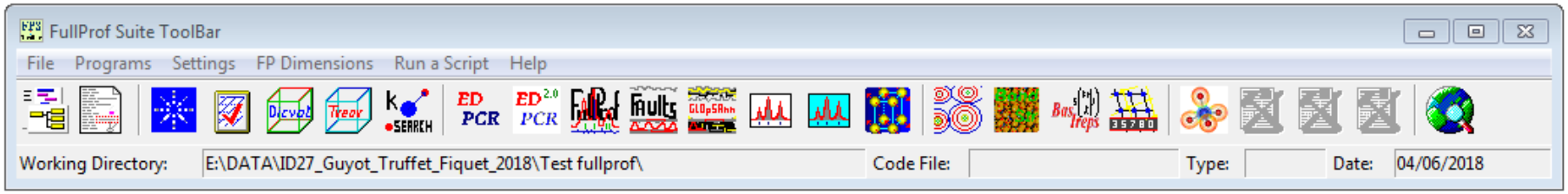
C	00-210-4748	Silicon [Silicon]	Si	0.97081	0.86807	1.0041	0.84697	35.1%	☑
C	00-900-7496	[Corundum]	Al2 O3	0.79487	0.72792	0.33675	0.83318	52.2%	☑
C	00 230 0375		Al2 O3	0.75590	0.25678	0.29407E 01	0.57545		
C	00-230-0448	aluminium oxide [corundum]	Al2 O3	0.73763	0.26246	0.29193E-01	0.57377	1.093	
C	00-151-1297	Pd3 Sm B	B Pd3 Sm	0.88690	0.85179E-01	0.20831E-01	0.54250	18.389	
C	00-900-8094	[Corundum]	Al1.82 Cr0.18 O3	0.71661	0.21103	0.28616E-01	0.53688	1.195	
C	00-900-6056	[Magnesiowuestite]	Fe0.4 Mg0.6 O	0.92201	0.19262	0.17368E-01	0.53572	4.239	
C	00-901-3247	[Periclase]	MgO	0.89999	0.16355	0.15658E-01	0.53105	3.202	

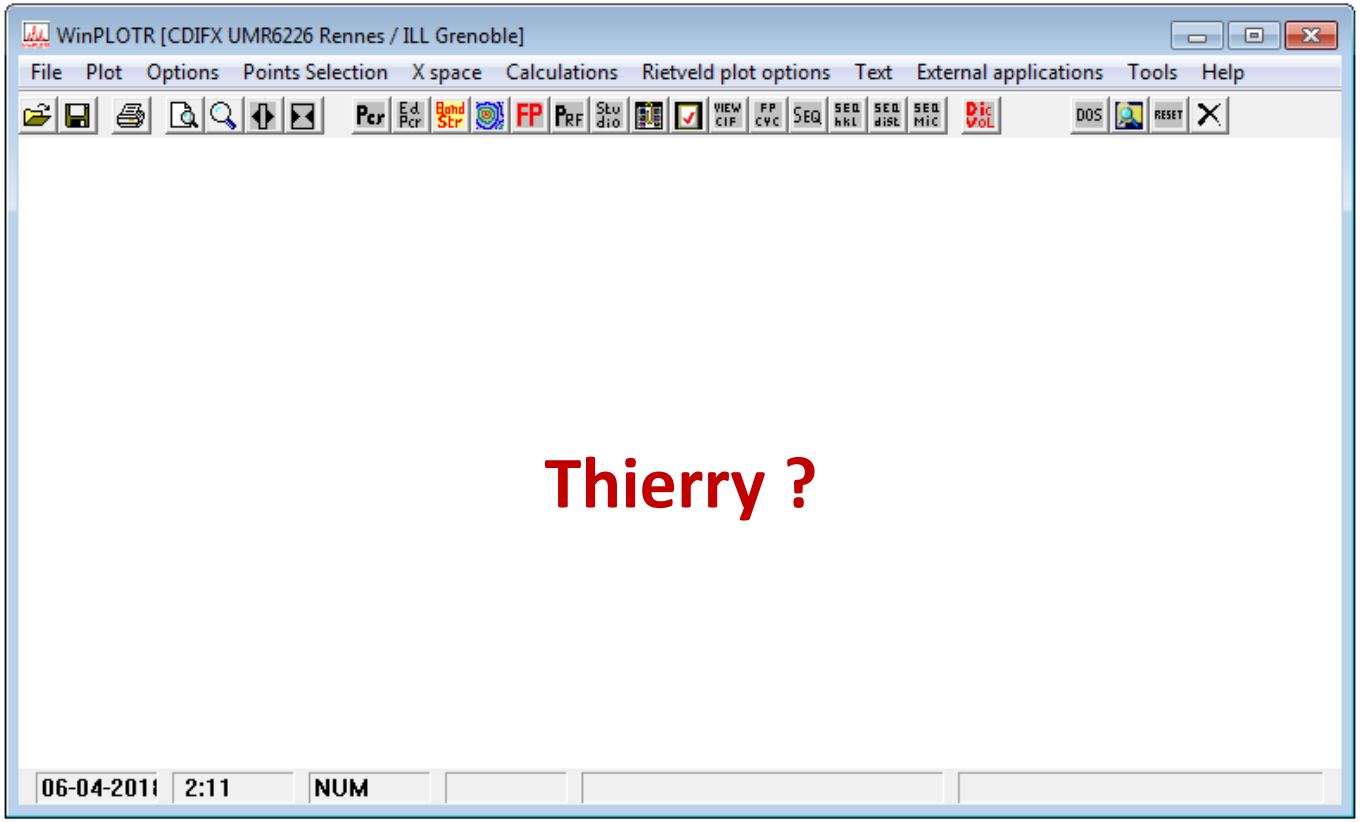
Matched POW_COD C 230 Selected Card 00-900-7496 Al2 O3

« Semi quantitative » estimation based on RIR

http://www.ba.ic.cnr.it/softwareic/qualx/

Phase identification using COD with Fullprof ?





Thierry ?

Phase identification using

Phase identification using

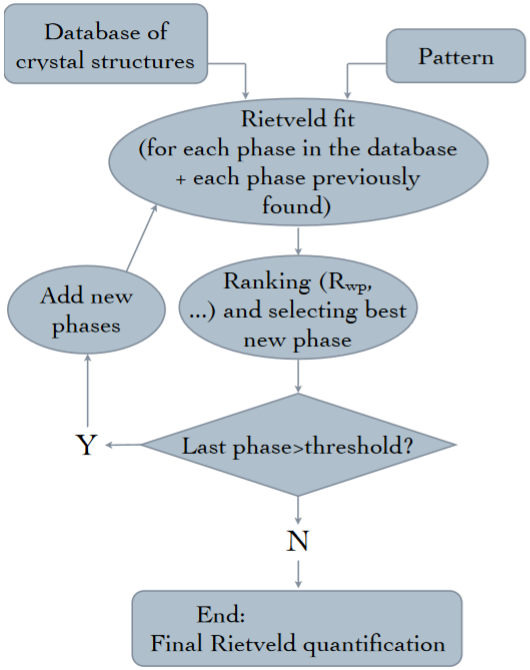
Full Profile Search Match
by L. Lutterotti using COD

http://nanoair.dii.unitn.it:8080/sfpm/
http://cod.iutcaen.unicaen.fr/

⇨ Search using an light version of the full COD (redundancies have been removed)

The FPSM (Full Pattern Search-Match method)

Developed inside the Nanoair project for the portable instrument



Pro:

- No user intervention, automatic analysis
- No peaks location/detection required (works with nano materials/particles)
- Full Rietveld quantitative analysis provided
- Works also for neutron and electron diffraction

Cons:

- Only phases with known crystal structure are ready to be used (unknown structures require a list of peaks and calibrated intensities, PONKS)
- Available databases are still incomplete
- If no elemental composition provided → requires > 20 minutes on 12 cores computer
- Good ranking algorithm required for very small phase amount

An open internet version has been setup at:
http://cod.iutcaen.unicaen.fr
http://nanoair.ing.unitn.it:8080/sfpm
search and quantification is limited by the time required (or better server response time) so it should be used restricting the composition as much as possible to speed up computation. A limited number of concurrent connections are supported also. INEL SAS can be inquired for the full version.

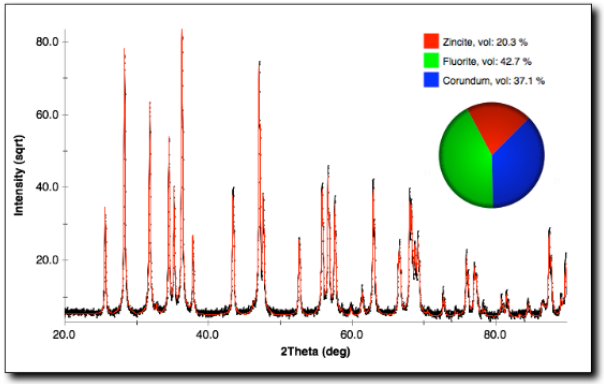
Full Profile Search Match

by L. Lutterotti using COD

what can we expect ?

Testing FPSM using the COD

Sample cpd1h from quantitative analysis Round-Robin
http://www.iucr.org/resources/commissions/powder-diffraction/projects/qarr



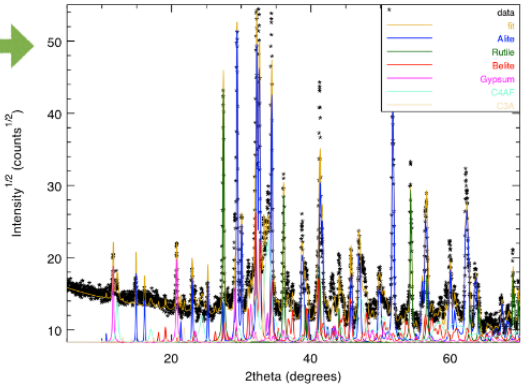
Phase (wt%)	FPSM	Round-Robin
ZnO	29	29.6
CaF	33.9	34.3
Al_2O_3	37.1	36.1

Total computation time (12 cores, 2.93GHz, COD, inorganic):

- No composition restriction: **565 secs**
- Only Al, Ca, F, Zn, O, Mg, Na, Si, Cl: **19 secs**

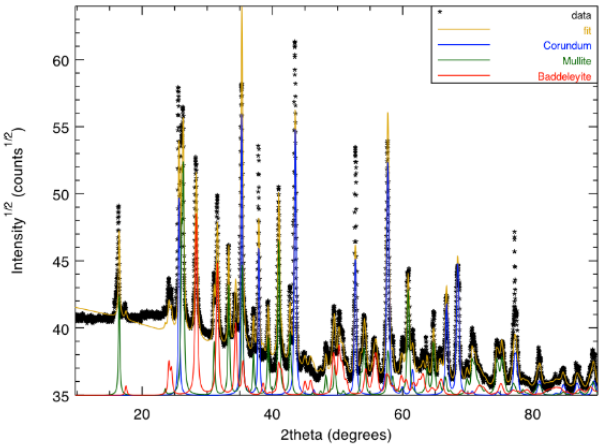
name	vol. (%)	wt. (%)	crystallites (A)	microstrain
Alite	52.3359	50.1148	2722.86	0.000913623
Rutile	8.7909	11.3199	1382.41	4.9784e-05
Belite	14.6584	14.8578	1014.1	0.00145265
Gypsum	7.28186	5.03503	881.992	0.00175863
C4AF	14.4548	16.3939	485.795	0.00705494
C3A	2.47814	2.27862	1426.2	0.00125916

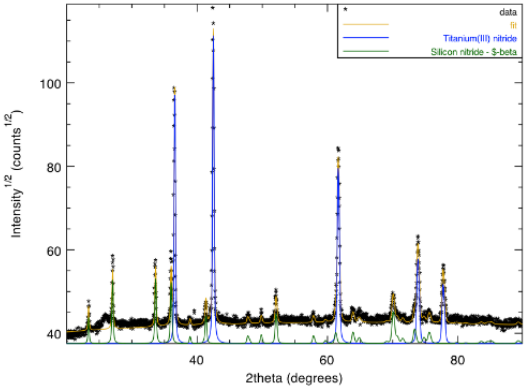
Some additional phases (cement phases) can been user added to the database if not present in the COD



Phase ID	name	vol. (%)	wt. (%)	crystallites (Å)	microstrain
9009672	Corundum	41.0726	45.1467	730.664	0.00137145
9005502	Mullite	53.5784	46.2318	515.483	0.000527227
9005833	Baddeleyite	5.34905	8.62151	371.805	0.00203445

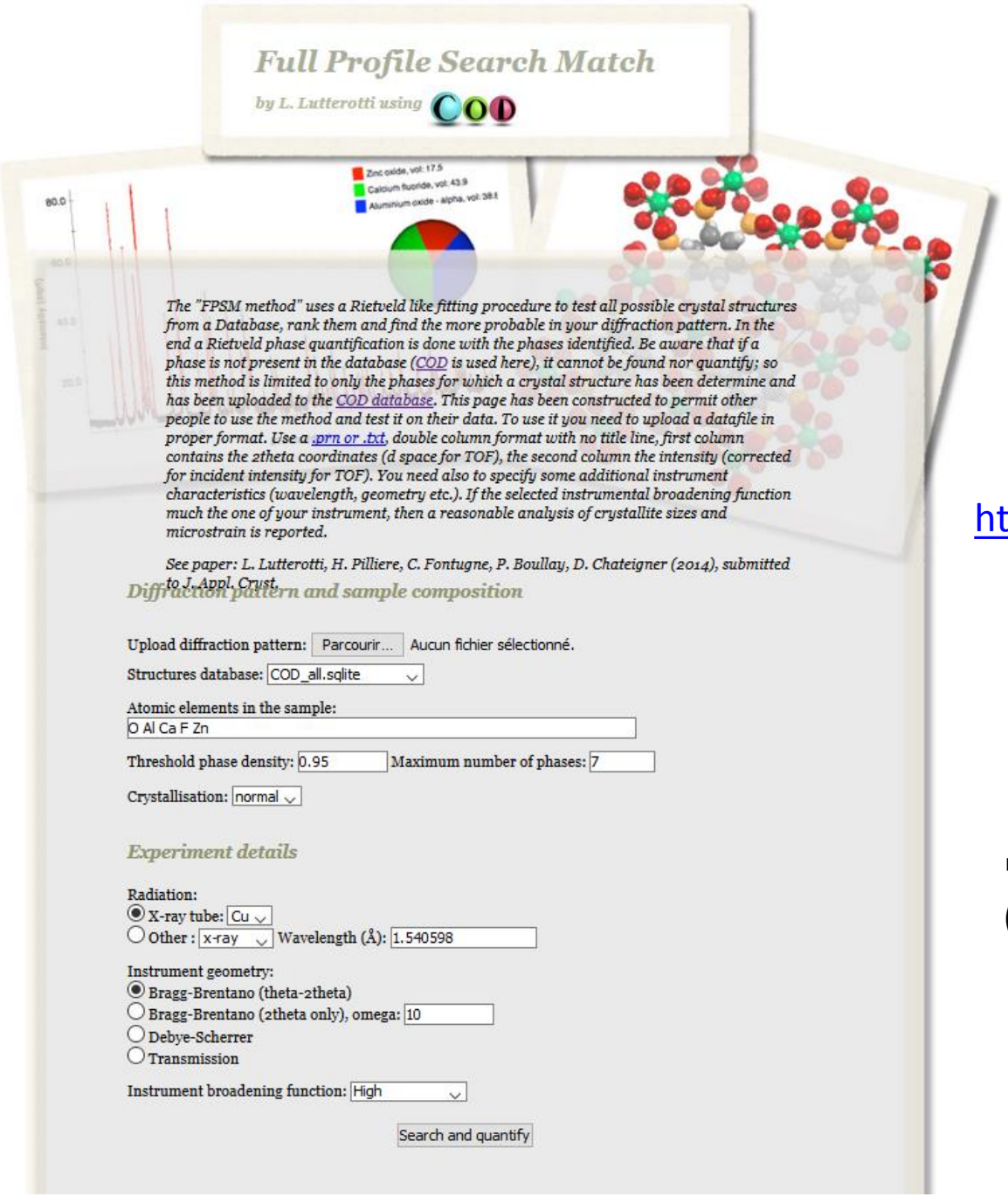
Final Rietveld analysis, Rw: 0.0455532, GofF: 1.79502





Phase ID	name	vol. (%)	wt. (%)	crystallites (Å)	microstrain
1101045	Titanium(III) nitride	50.0729	62.8891	1682.09	0.00122093
1001246	Silicon nitride - $-beta	49.9271	37.1109	800.99	0.00129495

Final Rietveld analysis, Rw: 0.0601521, GofF: 2.66024



2 web sites :

http://nanoair.dii.unitn.it:8080/sfpm/

http://cod.iutcaen.unicaen.fr/

Not directly from COD

⇨ light version of the full COD (redundancies have been removed)

demonstration

Input file : *.prn 2 columns : (2θ, Intensities)

148.400	49
148.420	43
148.440	36
148.460	37
148.480	46
148.500	39
148.520	47
148.540	33
148.560	43
148.580	50
148.600	44
148.620	37
148.640	44
148.660	39
148.680	37
148.700	54
148.720	46
148.740	43
148.760	39
148.780	56
148.800	28
148.820	32
148.840	32
148.860	42
148.880	50
148.900	51
148.920	49
148.940	53
148.960	64

…

http://nanoair.dii.unitn.it:8080/sfpm

How to obtain the COD ?

- The COD is a totally free of charge database and all its content can be downloaded :

  wiki.crystallography.net/howtoobtaincod/

- All the CIFs are accessible here :

  www.crystallography.net/cif/

main CIF donators

The American Mineralogist Crystal Structure Database

The main source of COD mineral data.

and

March 2003 and later, ~7000 CIFs

IPMC institut de physique de la matière condensée

April 2003, >1200 CIFs

Laboratoire LdF des Fluorures

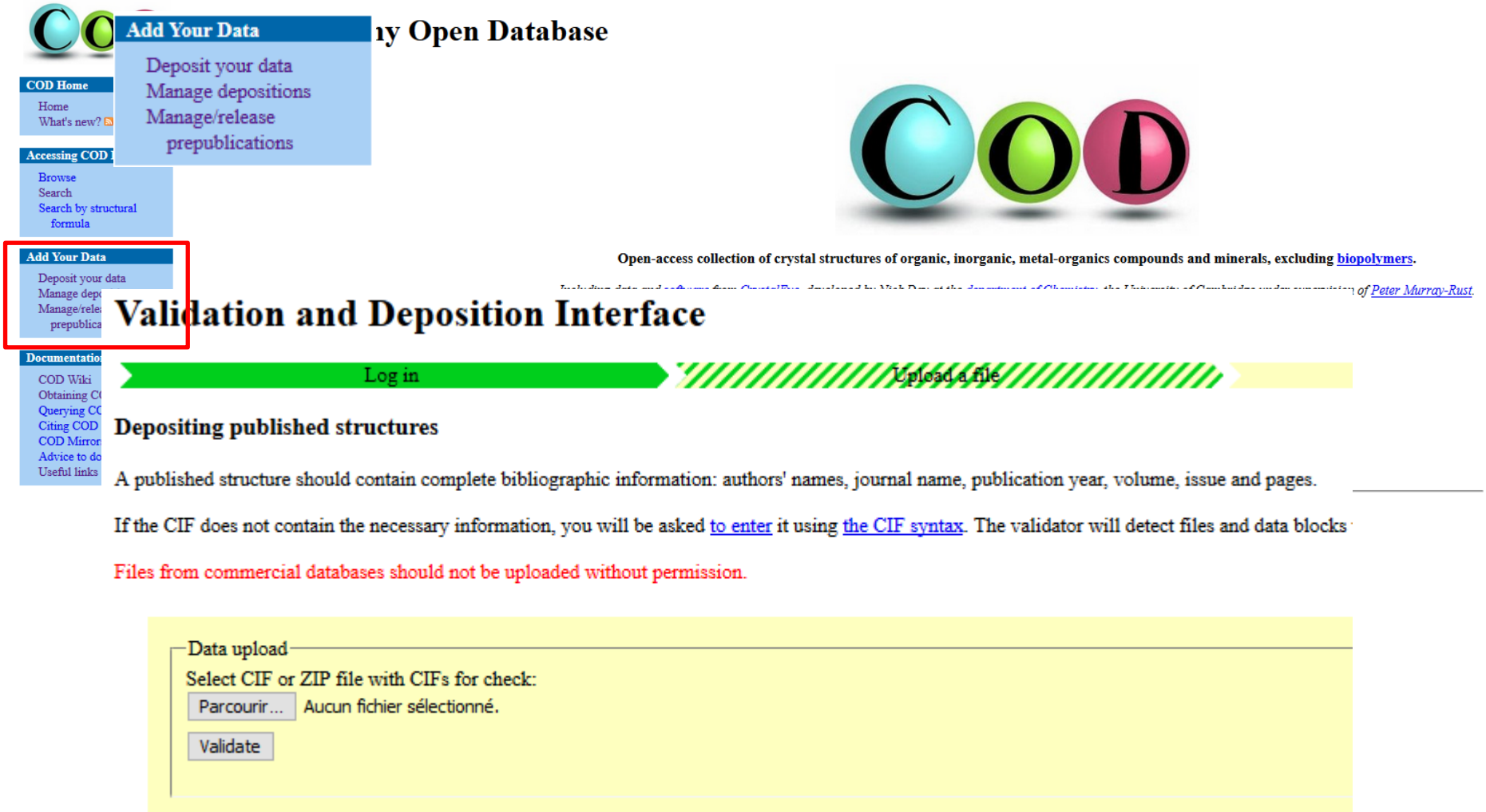
March 2003, > 450 CIFs

Laboratoire de Cristallochimie et
Physicochimie du Solide - CNRS UMR 8012 - Lille - France
> 100 CIFs

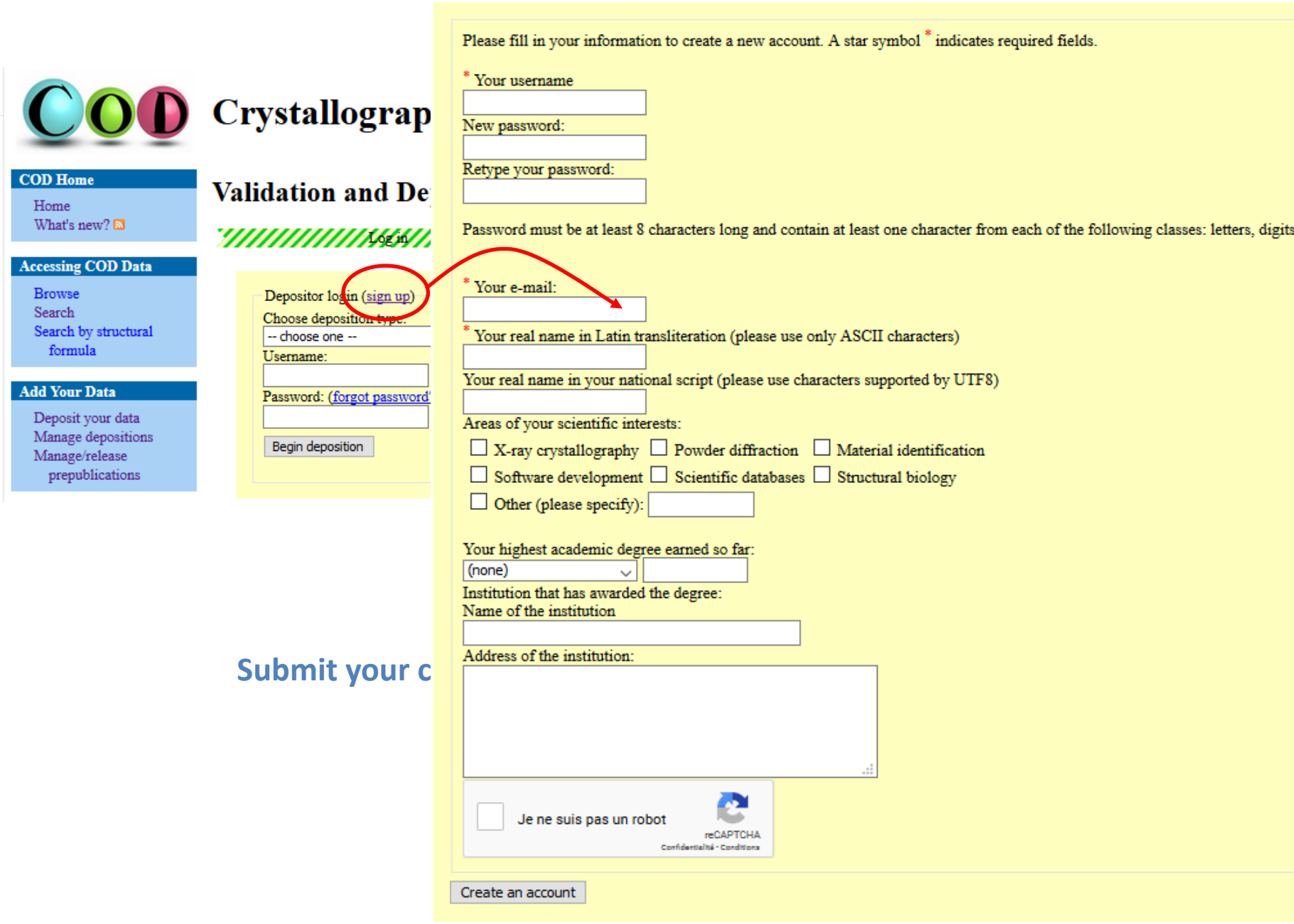
March 2003, > 850 CIFs

and … you !

How to contribute to the COD ?



But before, you need to create an account…



Submit your c

COD extensions …

TCOD : Theoretical Crystallography Open Database

www.crystallography.net/tcod/

- ✓ collection of theoretically calculated crystal structures
- ✓ organic, inorganic, metallorganic compounds and minerals
- ✓ 2764 entries

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mpod : Material Properties Open Database

http://mpod.cimav.edu.mx/

- ✓ .mpod file similar to .cif gathering the physical and chemical properties of materials

Search tool of mpod

mpod Material Properties Open Database

HOME SEARCH BY DOCUMENTATION ABOUT MPOD

PROPERTY
COMPOSITION
REFERENCES

Search by Property

Here a list of all the properties present in the database is given. Following the link associated to the property name you can view the properties details and the set of datafiles associated with the property.

name	tensor dimensions	units	units detail
dielectric permittivity relative epsrij	3,3	1	pure number
dielectric permittivity relative epsrijS	3,3	1	pure number
dielectric permittivity relative epsrijT	3,3	1	pure number
dielectric stiffness relative betrijS	3,3	10^-4	pure number
dielectric stiffness relative betrijT	3,3	10^-4	pure number
elastic TOEC stiffness cijk	6,6,6	GPa	giga Pascal
elastic compliance sij	6,6	10^-12.Pa^-1	pico Pascal^-1
elastic compliance sijD	6,6	10^-12.Pa^-1	pico Pascal^-1
elastic compliance sijE	6,6	10^-12.Pa^-1	pico Pascal^-1
elastic stiffness cij	6,6	GPa	giga Pascal
elastic stiffness cijD	6,6	GPa	giga Pascal
elastic stiffness cijE	6,6	GPa	giga Pascal
elastic stiffness cijS	6,6	GPa	giga Pascal
electric charge carrier concentration n	0	10^19 cm-3	atoms per cubic centimetre
electric coercive field Eci	3	kV.cm^-1	kilovolts per centimetre
electric remnant polarisation Pri	3	10^-6 Ohm.cm^-2	micro Ohm per square centimetre
electric resistivity rhoeij	3,3	10^-6 Ohm.cm	micro Ohm per centimetre
electromechanical coupling kij	3,6	1	pure number

Example of .mpod file :

- a standard part …
- … + a section dedicated to the properties

```
_phase_density ?
_prop_measurement_method '?'
_prop_conditions_magnetic_field ?
_prop_electric_resistivity_rhoeij 'rhoeij'
_prop_superconducting_critical_temperature_onset ?
_prop_superconducting_critical_temperature_onset_90 ?
_prop_superconducting_critical_temperature_mid_50 3.7
_prop_superconducting_critical_temperature_offset_10 ?
_prop_superconducting_critical_temperature_thermodynamic ?
_prop_superconducting_zero_resistivity_temperature ?
_prop_superconducting_resistivity_transition_width 0.1
_prop_superconducting_critical_field2_Hc2i 'Hc2i'
_prop_superconducting_critical_field1_Hc1i 'Hc1i'
_prop_superconducting_irreversibility_field_Hirri 'Hirri'
_prop_superconducting_coherence_length_ksii 'ksii'
_prop_superconducting_penetration_depth_lambdai 'lambdai'
_prop_residual_resistivity_ratio 12.4
_prop_residual_resistivity_ratio_high_temperature 300
_prop_residual_resistivity_ratio_low_temperature 4
loop_
_prop_data_label
_prop_data_tensorial_index
_prop_data_value
_prop_conditions_temperature
rhoeij 11 110 300
rhoeij 22 110 300
rhoeij 33 ? ?
rhoeij 11 8.9 4
rhoeij 22 8.9 4
rhoeij 33 ? ?
Hc1i 1 0.023 0
Hc1i 2 0.023 0
Hc1i 3 0.023 0
Hc1i 1 0.0114 1.8
Hc1i 2 0.0114 1.8
Hc1i 3 0.0100 1.8
Hc2i 1 0.114 0
Hc2i 2 0.114 0
Hc2i 3 0.114 0
Hirri 1 0.055 1.8
Hirri 2 0.055 1.8
Hirri 3 0.0544 1.8
ksii 1 54 0
ksii 2 54 0
ksii 3 54 0
lambdai 1 80 0
lambdai 2 80 0
lambdai 3 80 0
```

COD extensions …

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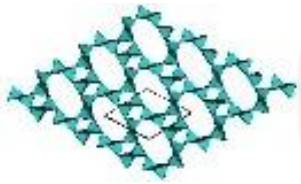

: Predicted Crystallography Open Database

http://www.crystallography.net/pcod/

- ✓ The PCOD is a subset of COD containing .cifs of inorganic structures candidates obtained from ZEFSA-II and GRINSP programs.
- ✓ The P2D2 (*Predicted Powder Diffraction Database*) contains the powder patterns of these predicted structures and allows a search match job using Eva (Bruker)
- ✓ 1062771 records

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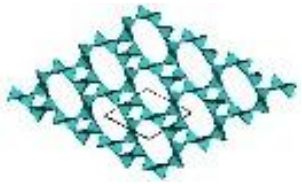

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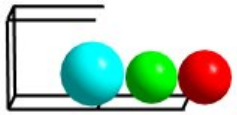

: Raman Open Database

http://solsa.crystallography.net/rod/

- ✓ The last one … from Daniel Chateigner & Yassine El Mendili
- ✓ 708 entries

Merci pour votre attention