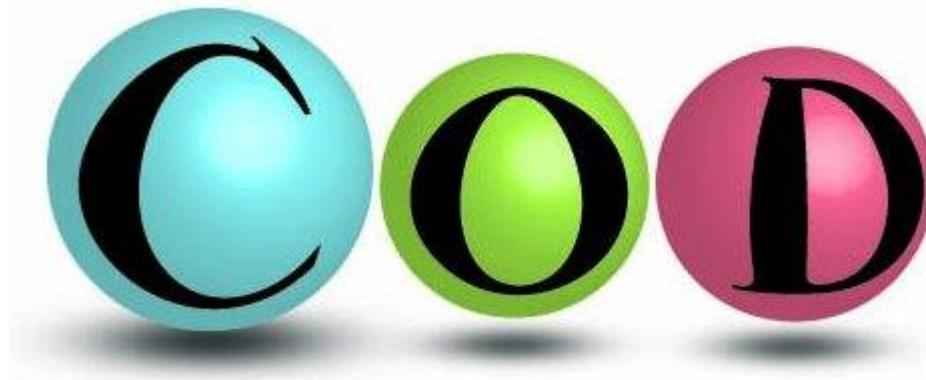


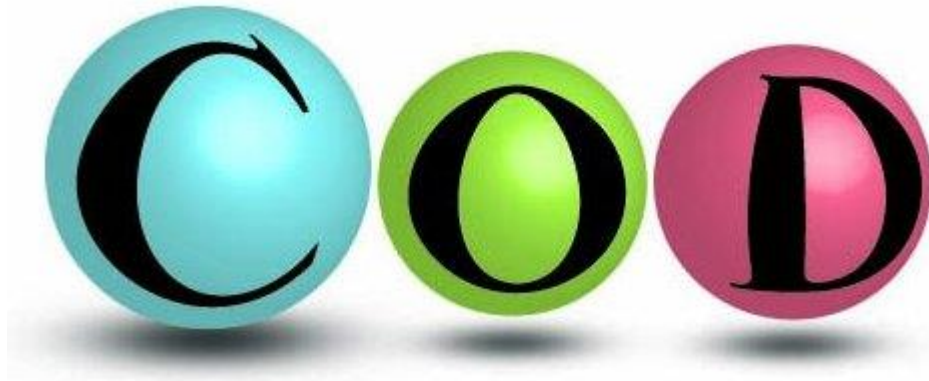
Un petit tour de la



Crystallography Open Database

avec Benoît Baptiste et Olivier Pérez

La



... et son environnement

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



<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

Crystallography databases : **money**



The Cambridge Crystallographic

<http://www.ccdc.cam.ac.uk/> (1965)

Organic

Compounds

bib
cnrs

<https://bib.cnrs.fr/>



FIZ Karlsruhe

ICSD

<http://www2.fiz-karlsruhe.de/icsd.html> (1978)

Inorganic

entries

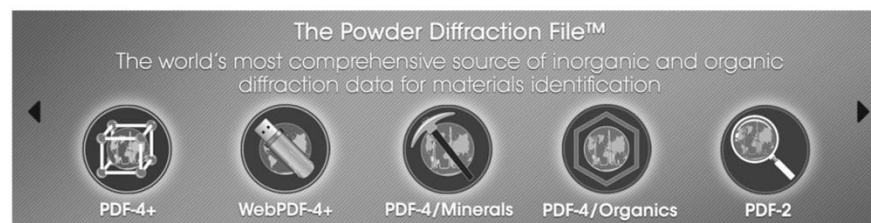
bib
cnrs

<https://bib.cnrs.fr/>

but INC only !



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Amorphous, poorly crystalline, nanomaterials disordered crystals

11300 raw diffraction patterns

bib
cnrs

<https://bib.cnrs.fr/>

soon ?

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

Crystallography databases : open access

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Biological macromolecules

X-ray, NMR & electron - 120000 entries

UA Mineralogy | Caltech Mineralogy



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

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

Crystallography databases : open access



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

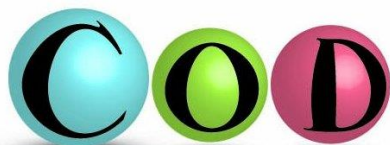
<https://www.rcsb.org/> (1971)



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

Biological macromolecules

X-ray, NMR & electron - 120000 entries



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

Organic, metal-organic, inorganic, minerals

X-ray, electron & neutron - 376000 records



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

Mineralogy Database

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

Organic, metal-organic, inorganic, minerals

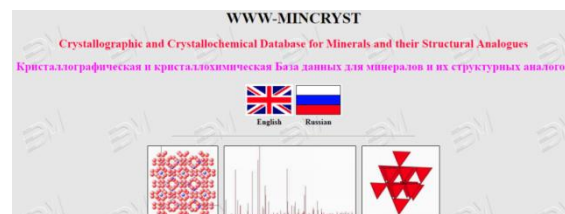
X-ray, electron & neutron - 376000 records



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

Mineralogy Database

<http://webmineral.com/> - 4700 entries

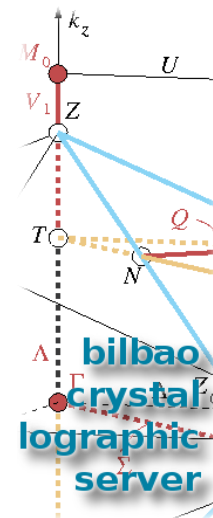


<http://database.iem.ac.ru/mincryst/> (1997) 9800 records

American Mineralogist Crystal Structure Database

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

Minerals



**Magnetic,
incommensurate
and modulated
structures**
148 entries

bilbao crystallographic server

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

Properties of crystallographic symmetry groups

Crystallography databases : open access

RCSB **PDB**
PROTEIN DATA BANK

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

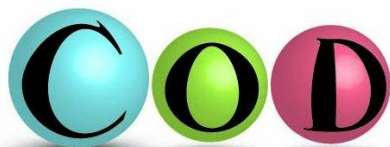
<https://www.rcsb.org/> (1971)

ndb NUCLEIC ACID
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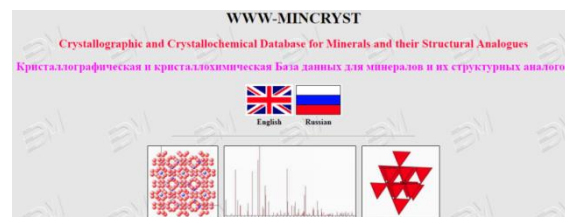
X-ray, electron & neutron - 376000 records



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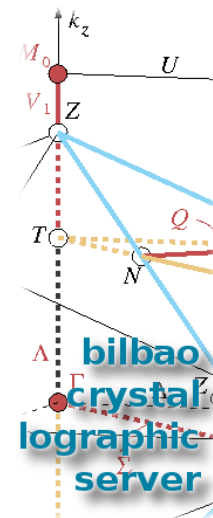


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bilbao crystallographic server

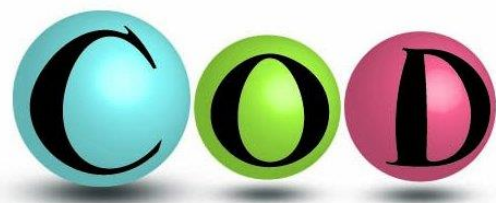
<http://www.cryst.ehu.es/> (1997)

Properties of crystallographic symmetry groups

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



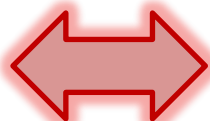
ndb NUCLEIC ACID
DATABASE

To improve the
description of ligands
for macromolecules



The Cambridge Crystallographic
Data Centre

To propose shared
services in all
chemistry domains



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/I₀), 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, $2\Theta = 2(\arcsin(n\lambda/(2d)))$ 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 1.54056 - CuK α 1	Change X-Ray λ ▼	D ₁ Å 3.34	D ₂ Å 	D ₃ Å 	Tolerance % 10	Elements SiO ₂	Validator
--	-----------------------------	--------------------------	----------------------	----------------------	-------------------	------------------------------	-----------

Listing of 6 Records Sorted by D₁ using 1.54056 - CuK α 1 for 2 Θ WHERE (d1 > 3.006 AND d1 < 3.674) AND (formula LIKE 'SiO2')

D ₁ Å (2 Θ)	I ₁ (%)	D ₂ Å (2 Θ)	I ₂ (%)	D ₃ Å (2 Θ)	I ₃ (%)	Mineral	Formula
3.098(28.79)	100	3.432(25.94)	50	2.770(32.29)	15	Coesite	SiO ₂
3.335(26.71)	100	4.430(20.03)	90	3.391(26.26)	58	Moganite	SiO ₂
3.342(26.65)	100	4.257(20.85)	22	1.818(50.14)	14	Quartz	SiO ₂
3.390(26.27)	50	1.370(68.42)	100	1.380(67.86)	100	Lutecite	SiO ₂
3.390(26.27)	50	1.380(67.86)	100	1.370(68.42)	100	Lutecite	SiO ₂
3.390(26.27)	50	1.380(67.86)	100	1.830(49.79)	100	Lutecite	SiO ₂

a quick search with 3 peaks

Open database : **AMCSD** example

American Mineralogist Crystal Structure Database

This site is an interface to a crystal structure database that includes every structure published in the American Mineralogist, The Canadian Mineralogist, European Journal of Mineralogy and Physics and Chemistry of Minerals, as well as selected datasets from other journals. The database is maintained under the care of the Mineralogical Society of America and the Mineralogical Association of Canada, and financed by the National Science Foundation.

	<u>Mineral</u>
	<u>Author</u>
	<u>Chemistry Search</u>
	<u>Cell Parameters and Symmetry</u>
	<u>Diffraction Search</u>
	General Search
	<u>Search Tips</u>
Search Reset	

Logic interface	☒ AND ☐ OR
Viewing (About File Formats)	☒ amc long form ☐ amc short form ☐ cif
Download	☒ amc ☐ cif ☐ diffraction data

People



Extra

Open database : AMCSD example

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benitoite

Mineral

Author

Chemistry Search

Cell Parameters and Symmetry

Diffraction Search

General Search
Search Tips

short form ☐ cif

on data

Mineral Index: A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

Babephite	Batisvite	Berzelianite	Bobfergusonite	Brezinaite
Babingtonite	Baumhauerite	Berzeliite	Bobierite	Brianite
Baddeleyite	Baumstarkite	Beshtauite	Bobjonesite	Brianroulstonite
Bafertisite	Bavenite	Beta - fergusonite-(Ce)	Bobkingite	Briartite
Baghdadite	Bayerite	Beta - fergusonite-(Y)	Bobmeyerite	Bridgmanite
Bahianite	Bayldonite	Beta-diopside	Bobtraillite	Britholite
Bairdite	Bayleyite	Beta-roselite	Bogdanovite	Britholite-(Ce)
Bakerite	Baylissite	Beta-sulfur	Boggildite	Britholite-(Gd)
Bakhchisaraitsevite	Bazhenovite	Betafite	Boggsite	Britholite-(La)
Baliczunicite	Bazirite	Betalomonosovite	Bohdanowiczite	Britholite-(Y)
Balipholite	Bazzite	Betekhtinite	Bohmite	Britvinite
Balliranoite	BC-8	Betpakdalite-CaCa	Boleite	Brizziite
Balyakinite	Bearsite	Betpakdalite-CaMg	Boltwoodite	Brochantite
Bamfordite	Bearthite	Beudantite	Bonaccordite	Bromargyrite
Banalsite	Beaverite	Beusite	Bonattite	Bromcarnallite
Bandylite	Beaverite-(Cu)	Beyerite	Bonazzite	Bromellite
Bannermanite	Beaverite-(Zn)	Bicchellaite	Bonshtedtite	Bromine
Bannisterite	Bechererite	Bianchite	Boracite	Brontesite
Baotite	Becquerelite	Bicchulite	Borasilite	Brookite
Bararite	Bederite	Bideauxite	Borax	Browneite
Baratovite	Behierite	Bieberite	Borcarite	Brownleeite
Barberiite	Behoite	Biehlite	Bornemanite	Brownmillerite
Barbertonite	Behounekite	Bigcreekite	Bornite	Brucite
Barboselite	Belakovskite	Bijvoetite-(Y)	Borodaevite	Bruggenite
Barentsite	Belendorffite	Bikitaite	Boromullite	Brunogeierite
Baricite	Belkovite	Billietite	Boromuscovite	Brushite



Extra

Open database : **AMCSD** example

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benitoite

Mineral

Author

Chemistry Search

alpha=90(0) and Cell Parameters and Symmetry

tolerance(0.02),inte Diffraction Search

General Search

Search Tips

Search Reset

OR

g form ☐ amc short form ☐ cif

cif ☐ diffraction data

Periodic Table

1 H																	2 He				
3 Li	4 Be															5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg															13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr				
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe				
55 Cs	56 Ba	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu					
87 Fr	88 Ra	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr					

go

D

go

Wat

go

OH

Search Selected Elements

Open database : **AMCSD** example

American Mineralogist Crystal Structure Database

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Cell Parameters and Symmetry

	Value	Tolerance	
a	6.64	0.05	☐ Range
b	6.64	0.05	☒ Tolerance
c	9.77	0.05	
alpha	90	0	
beta	90	0	
gamma	120	0	
space group			
crystal system	hexagonal		

Logic interface:
☒ AND ☐ OR

☒ AND ☐ OR
☐ amc long form ☐ amc short form ☐ cif
☒ amc ☐ cif ☐ diffraction data



Open database : **AMCSD** example

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Diffraction Pattern Search/Match Routine

Choose an option:

☒ d-spacing ☐ 2-theta ☐ Energy

Intensity Cutoff

d-spacing

Tolerance

0.05

Enter Values Above...

2.69 to 2.79
3.67 to 3.77
5.7 to 5.8

benitoite

Mineral

Author

Chemistry Search

Cell Parameters and Symmetry

Diffraction Search

General Search

Search Tips

AND ☐ OR

amc long form ☐ amc short form ☐ cif

amc ☐ cif ☐ diffraction data

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benitoite	Mineral
Miletich	Author
(Si,O,Ba,Ti)	Chemistry Search
a=6.64(5) and b=6.64(5) and c=9.77(5) and alpha=90(0) and	Cell Parameters and Symmetry
vals(2.74,3.72,5.75),opt(),type(d-spacing),tolerance(0.02),inte	Diffraction Search
	General Search
	Search Tips
Search Reset	

Logic interface	☒ AND ☐ OR
Viewing (About File Formats)	☒ amc long form ☐ amc short form ☐ cif
Download	☒ amc ☐ cif ☐ diffraction data

People



Extra

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, BaTiSi3O9, 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
----	-------	-------	-------	-------

[Download AMC data \(View Text File\)](#)

[Download CIF data \(View Text File\)](#)

[Download diffraction data \(View Text File\)](#)

[View Jmol 3-D Structure \(permalink\)](#)

Download in:

Multiple datasets can be concatenated into a single downloadable file by selecting the datasets and then clicking

Multiple datasets can be downloaded as individual files inside a ZIP archive by selecting the datasets and then clicking

Total number of retrieved datasets: **1**

View in **amclongform**, download in **amc**

Open database : AMCSD example

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Total number of retrieved datasets: 1

View in **amclongform**, download in **amc**

Cif file

```
data_global
_chemical_name_mineral 'Benitoite'
loop_
  _publ_author_name
    'Hejny C'
    'Miletich R'
    'Jasser A'
    'Schouwink P'
    'Crichton W'
    'Kahlenberg V'
  _journal_name_full 'American Mineralogist'
  _journal_volume 97
  _journal_year 2012
  _journal_page_first 1749
  _journal_page_last 1763
  _publ_section_title
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    Second-order P6c2-P31c transition and structural crystallography of
    the cyclosilicate benitoite, BaTiSi3O9, at high pressure
    Note: P = 0.0001 GPa
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  _cell_length_b 6.6430
  _cell_length_c 9.7660
  _cell_angle_alpha 90
  _cell_angle_beta 90
  _cell_angle_gamma 120
  _cell_volume 373.229
  _exptl_crystal_density_diffrn 3.679
  _symmetry_space_group_name_H-M 'P -6 c 2'
loop_
  _space_group_symop_operation_xyz
    'x,y,z'
    'x,x-y,-z'
    '-x+y,-x,1/2-z'
    '-y,-x,1/2+z'
```

Open database : AMCSD example

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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

[Download AMC data \(View Text File\)](#)

[Download CIF data \(View Text File\)](#)

[Download diffraction data \(View Text File\)](#)

[View Jmol 3-D Structure \(permalink\)](#)

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Diffraction data

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Note: P = 0.0001 GPa

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_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



: 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



[CIFs Donators](#)



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Daniel Chateigner, Xiaolong Chen, Marco Ciriotti,
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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



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Growing field of applications :

- Teaching [J. Appl. Cryst. \(2015\). 48, 1964-1975](#)
- 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

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 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

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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	
Reset	Send	



Crystallography Open Database : basic search

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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	
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 , <i>53</i> , 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 , <i>53</i> , 6034-6041



Crystallography Open Database : be an artist

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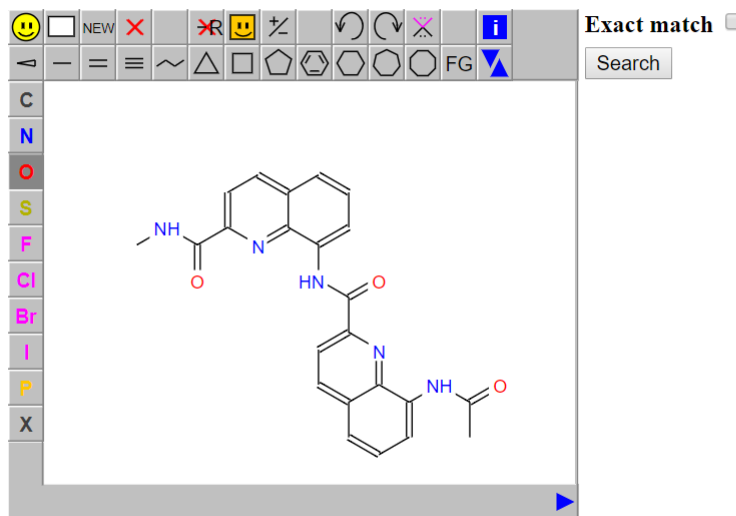
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Draw a structure or a fragment to search in COD



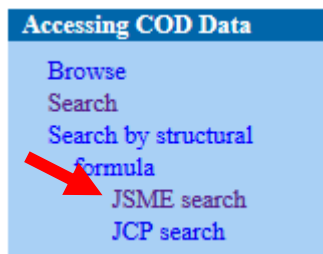
[Use JME search](#)

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

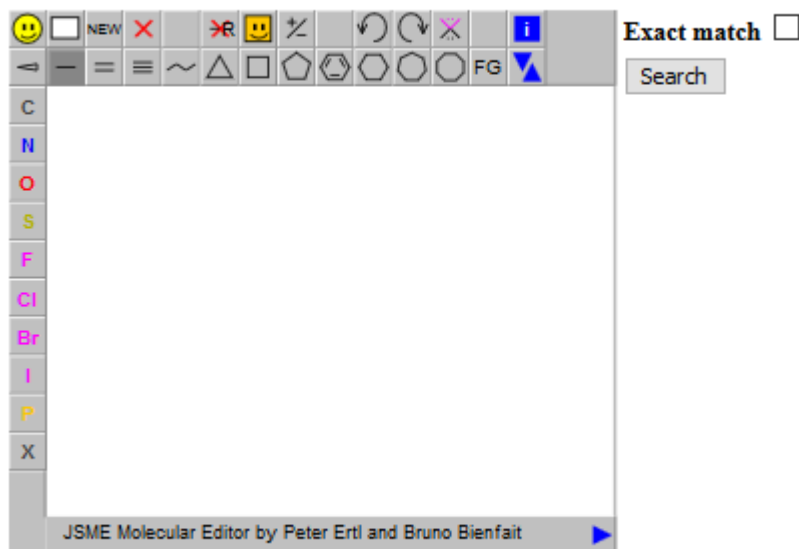
Just 1 result ?

COD ID ▲	Links	Formula ▲	Space group ▲	Cell parameters	Cell volume ▲	Bibliography
4120055	CIF HKL	C ₁₄₆ H ₁₈₀ N ₂₀ O ₂₄ 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 <i>Journal of the American Chemical Society</i> , 2013 , <i>135</i> , 9628-9631

Live search ...



Draw a structure or a fragment to search in COD



[Use JME search](#)

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

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



: also compatible with search and match programs

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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 submitted 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



: also compatible with search and match programs

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- **July 2016:** A new release of the COD-based search-match database is [available](#) from [PANalytical](#). → **HighScore(Plus)**
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What's New?

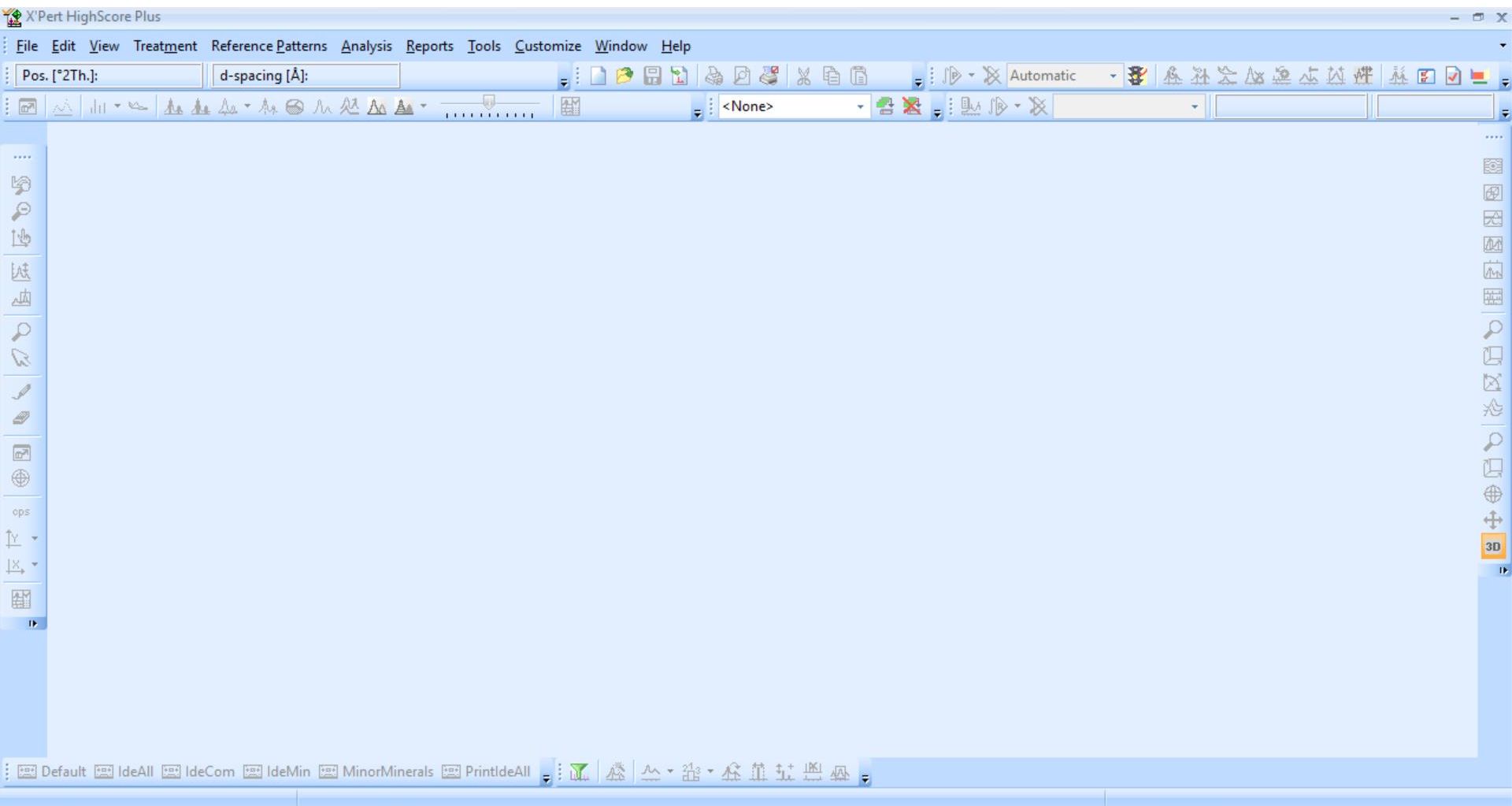
- September 2006: Thomas Holder ([author](#)) has released a new version of the [DataScribe](#) program which now allows to carry out structure search queries in the regular subset of the COD.
- July 2006: A new release of the COD-based search-match database is [available](#) from [Rorix](#).
- **July 2016: A new release of the COD-based search-match database is [available](#) from [PANalytical](#).** → **HighScore(Plus)**
- September 2005: Thomas Holder now offers the [source code](#) of the [COD database](#) for download on his [website](#).
- April 2005: Thomas Holder from [author](#) has released the [DataScribe](#) program in open source!
- November 2004: The [CODmatch](#) was a Rorix-like listing procedure to test all possible crystal structures from the Crystallography Open Database, rank them and find the most probable to your diffraction pattern. In the end a Rorix-like phase identification is done with the phase identified. The new paper is included in the 3. April 2005.
- November 2004: The new [CODmatch](#) version has been developed that can use COD data for search-match material identification.
- February 2003: Creation of the [COD](#) - Predicted Powder Diffraction Database (2003) entries - search-match possible with the EVA Broker software.

Download the archive for your commercial or open program

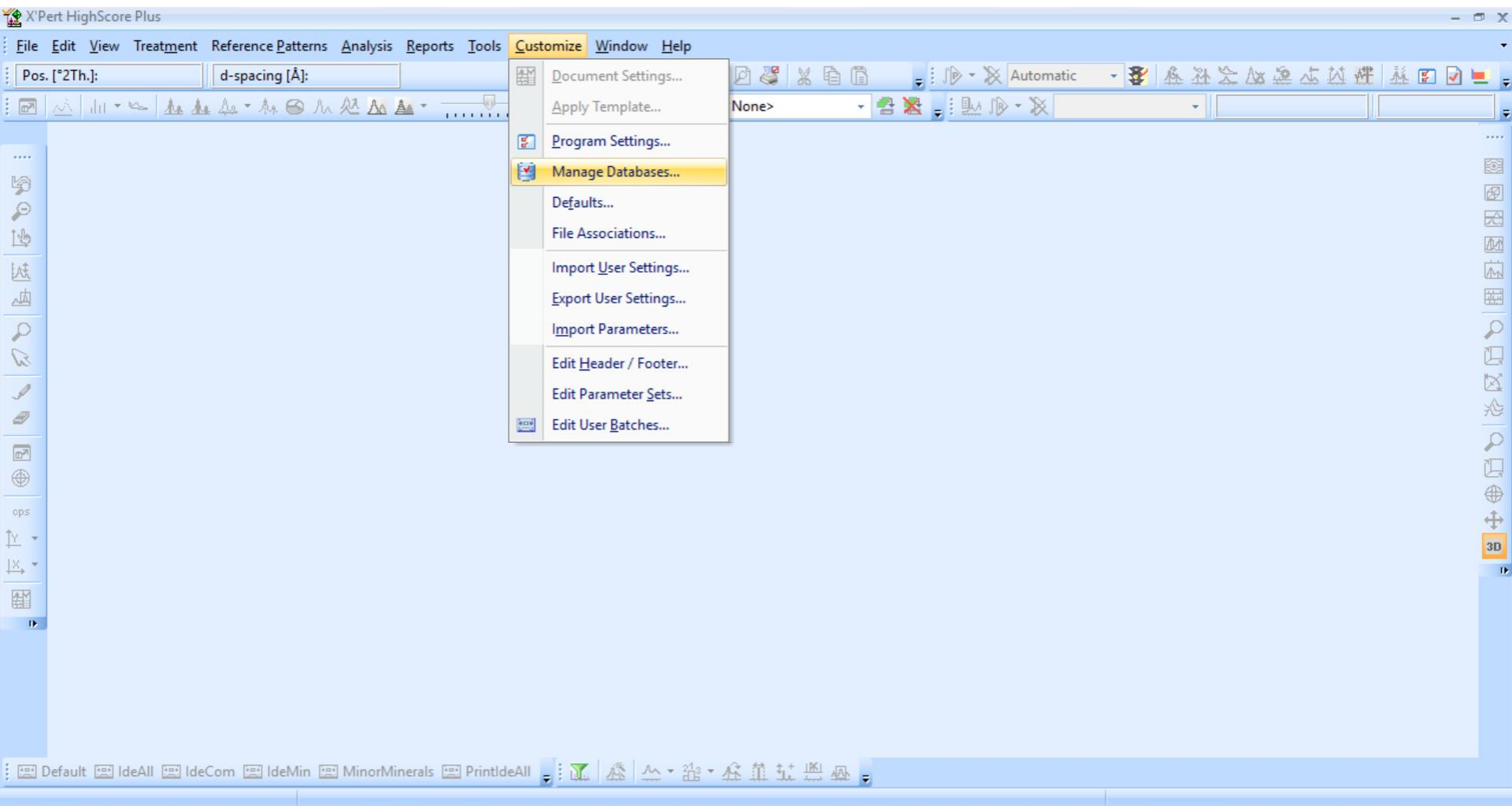
Index of /cod/archives/2016/PANalytical

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 with HighScore(Plus)



Phase identification using with HighScore(Plus)



Phase identification using with HighScore(Plus)

X'Pert HighScore Plus - [example1]

Pos. [°2Th.]: 104,763 d-spacing [Å]: 0,9725

Automatic

Manage Databases

Database Name	Use	Database Location	Content Type	Properties	Convert	Writable	Database Type
PANalytical Example Database	☐	C:\Program Files (x86)\PANalytical\X'Pert HighScore Plus\	PDF2 flat file	...	...		HighScore(Plus) V2.X database
PDF-2 Release 1995	☒	C:\Users\Baptiste\Desktop\pdf 2 1995 convert\	PDF2 flat file	...	...		HighScore(Plus) V2.X database
COD_2016_Conv45	☒	C:\Users\Baptiste\Documents\xrd_databases\COD_2016_	Converted CIF files	...		☐	HighScore(Plus) V3.X database

Counts

example1

1000

500

0

20 30

Total Number of Patterns: 431614

PDF-2 ...e 1995 73011

COD_2016_Conv45 358603

Disk Usage

Local

D:/

C:/

0 500 1 000 1 500 2 000 2 500

Gigabyte

Add HighScore Database...

Search for databases

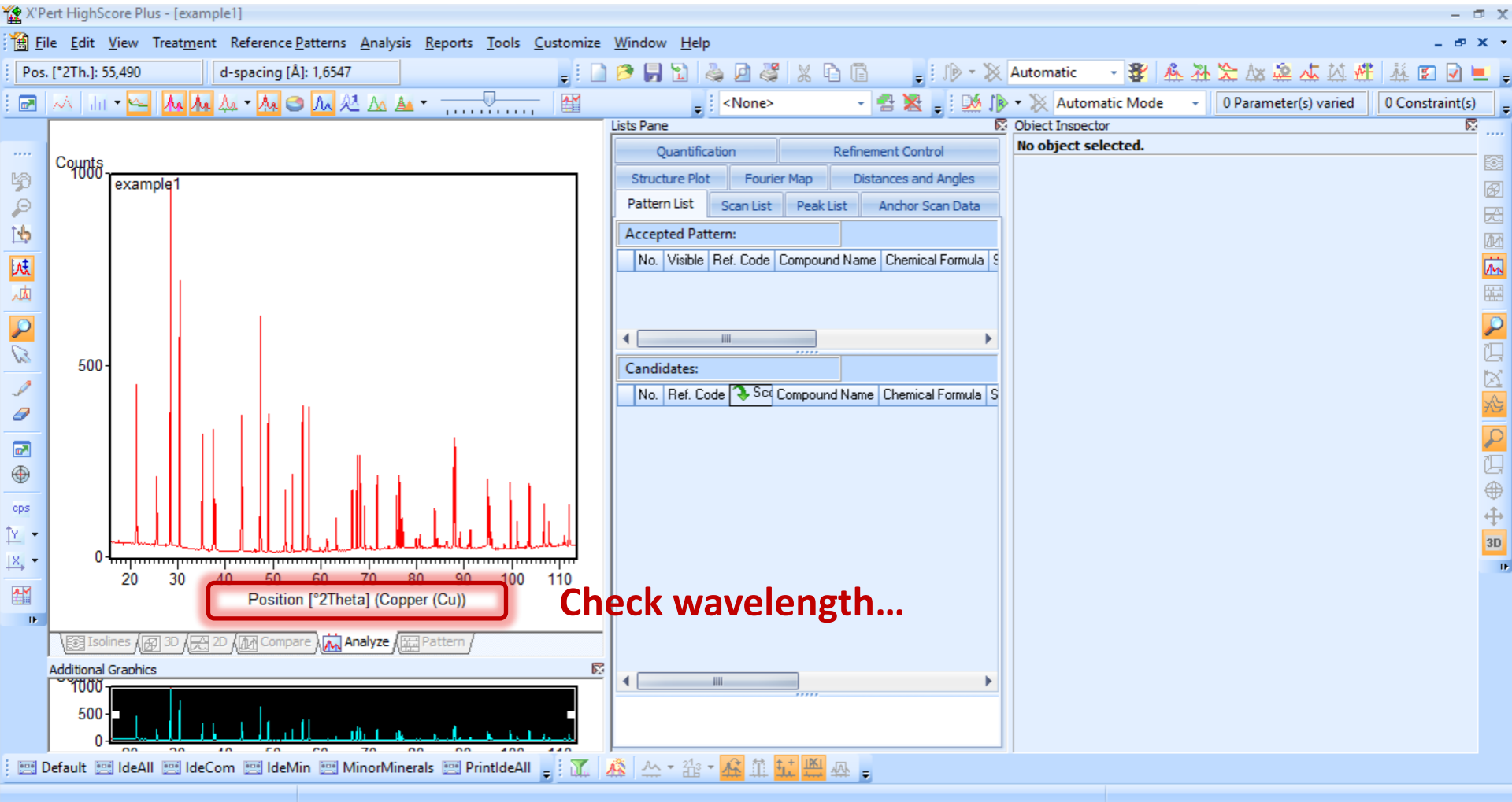
Create new empty database...

OK Cancel

Default IdeAll IdeCom IdeMin MinorMinerals PrintIdeAll

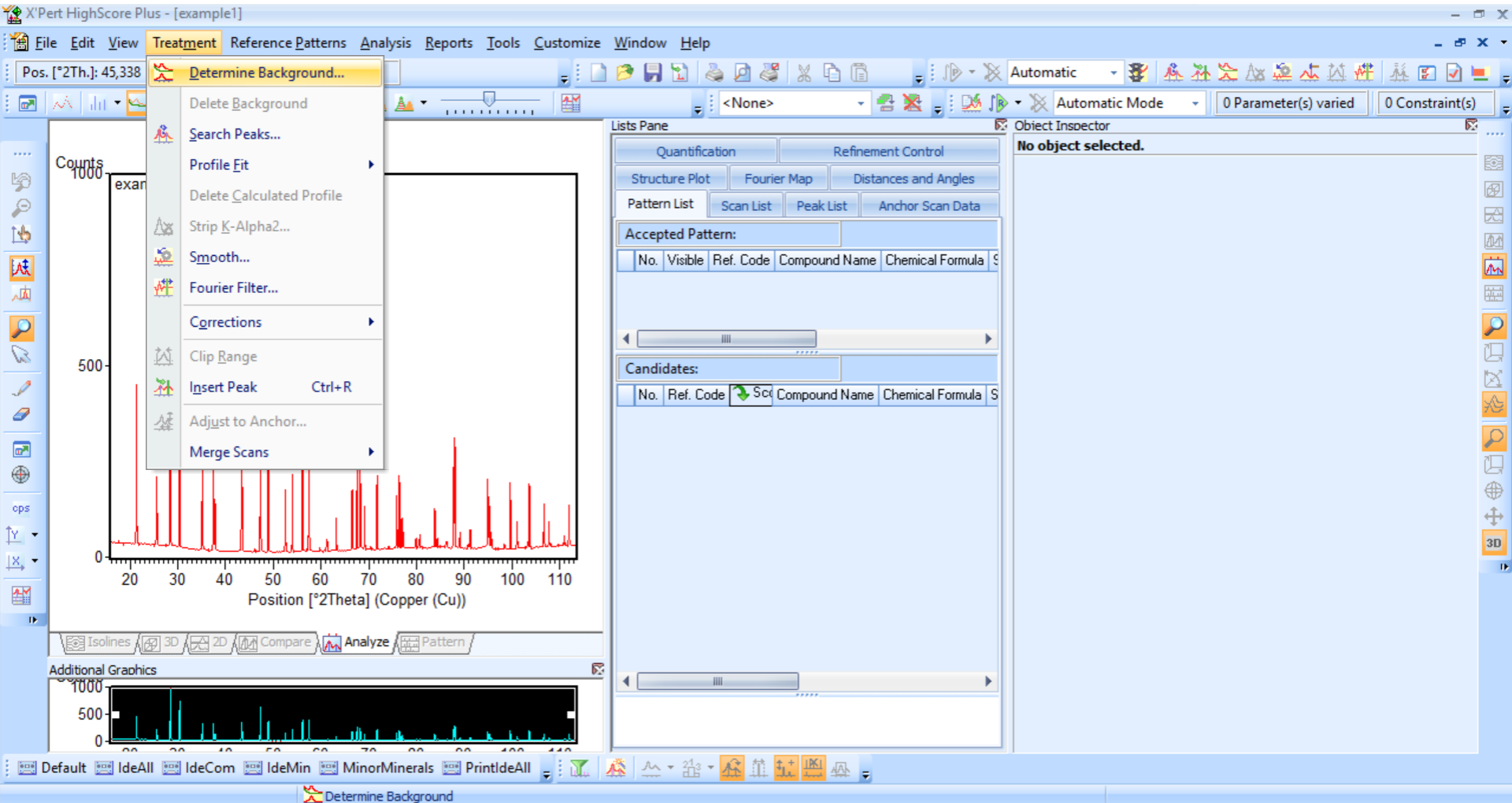
Phase identification using COD with HighScore(Plus)

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

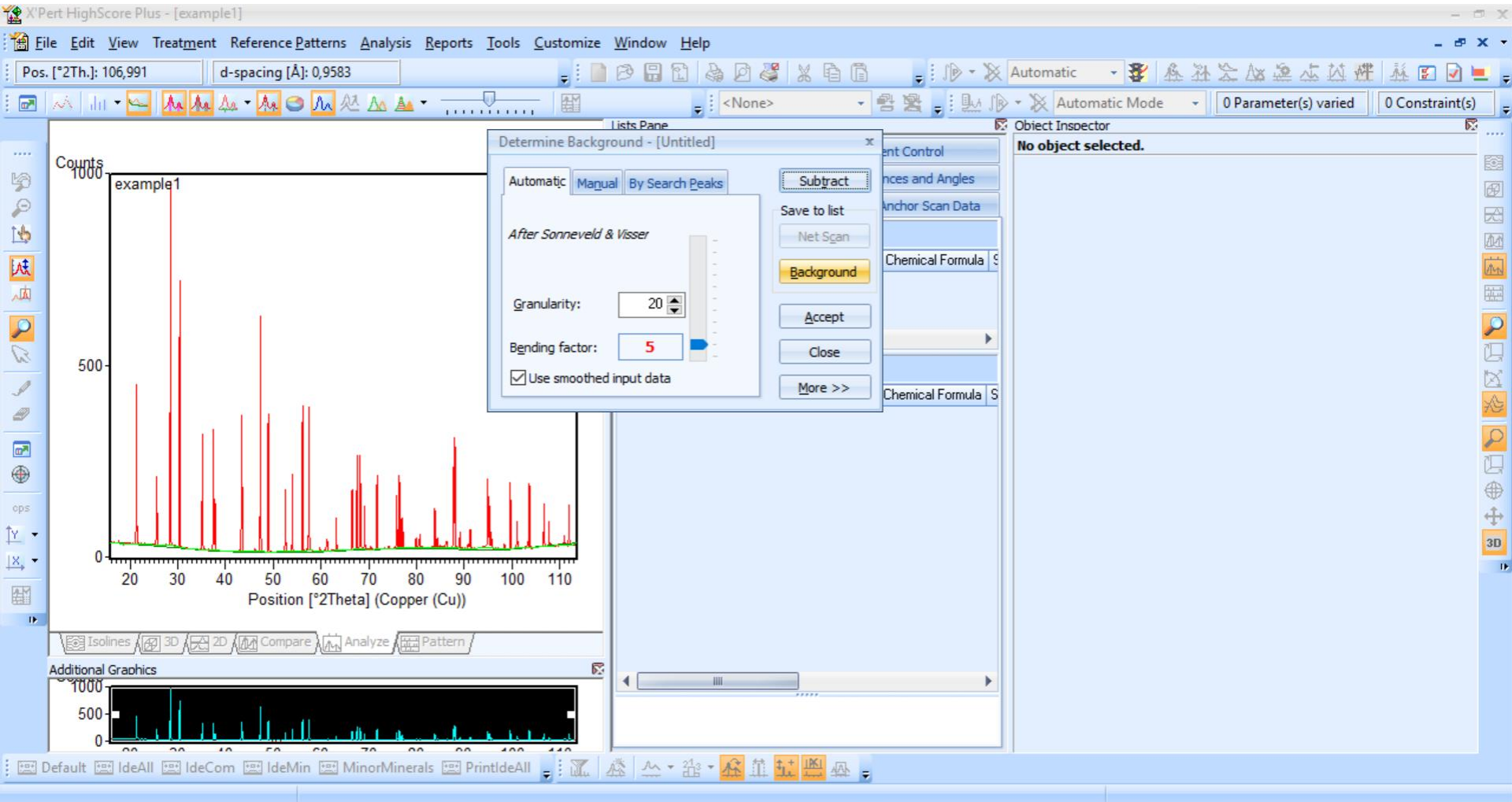


Phase identification using COD with HighScore(Plus)

Classical procedure : first model a bgd

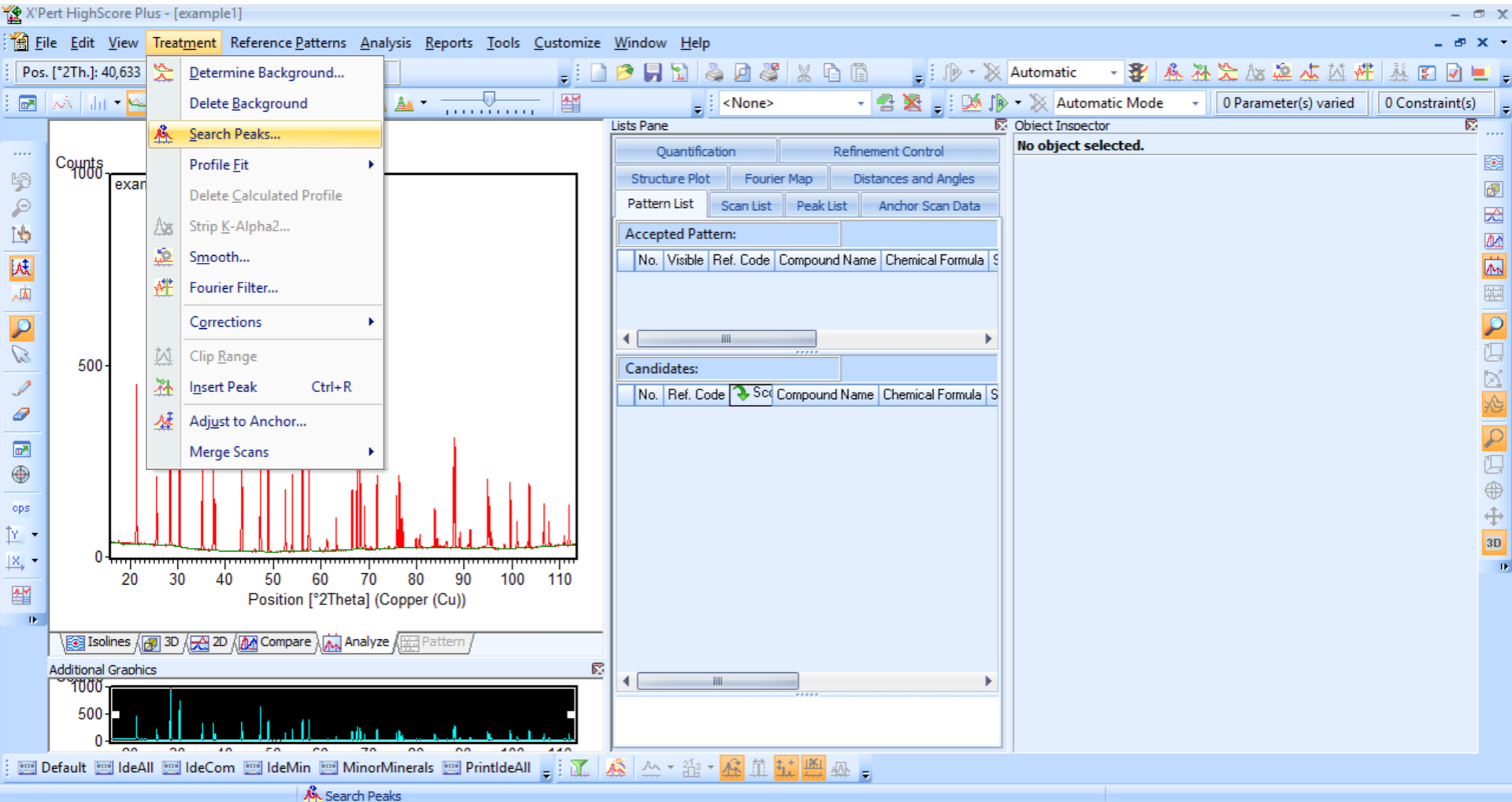


Phase identification using COD with HighScore(Plus)



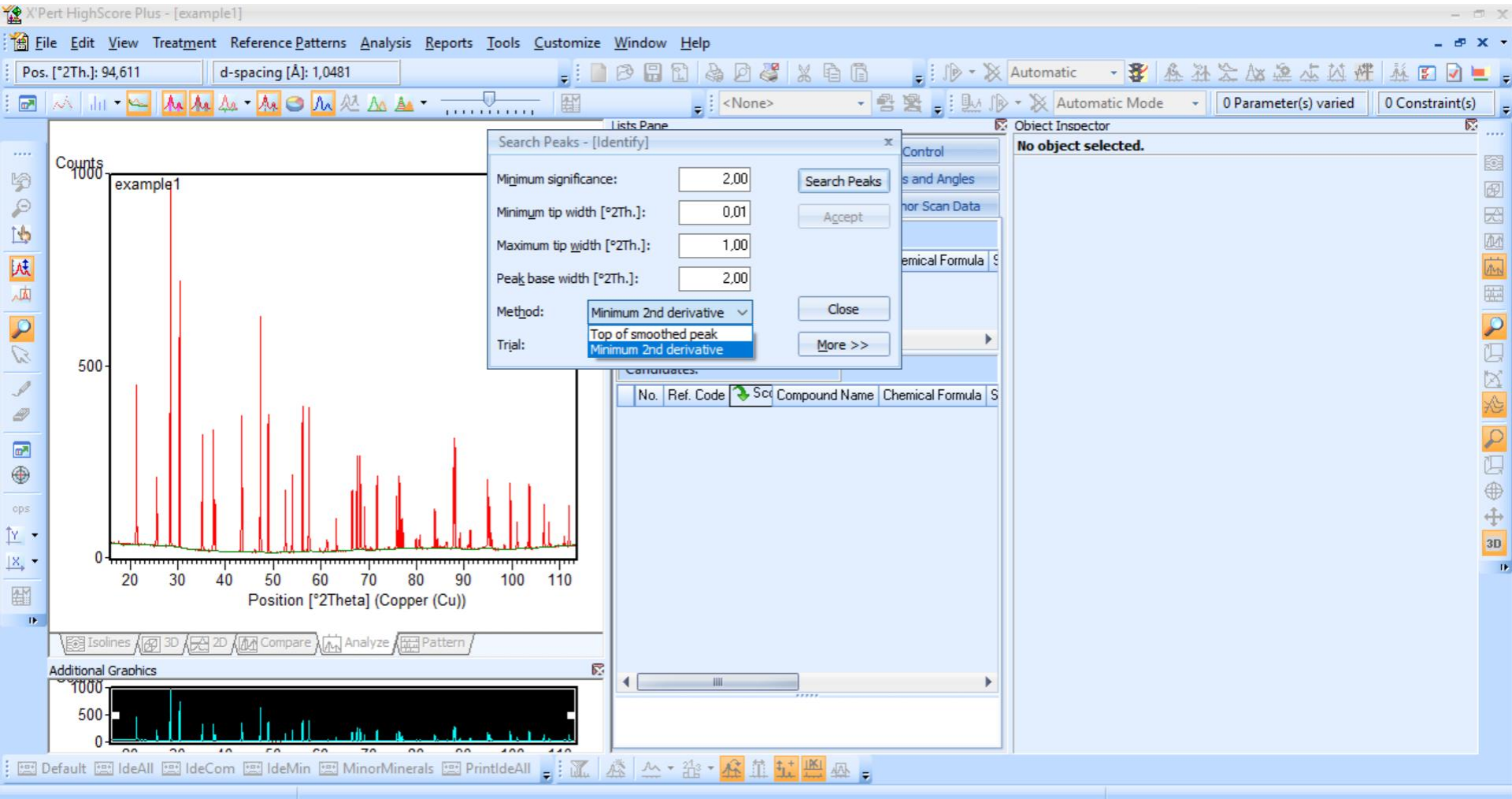
Phase identification using COD with HighScore(Plus)

Classical procedure : first model a bgd and then search peak



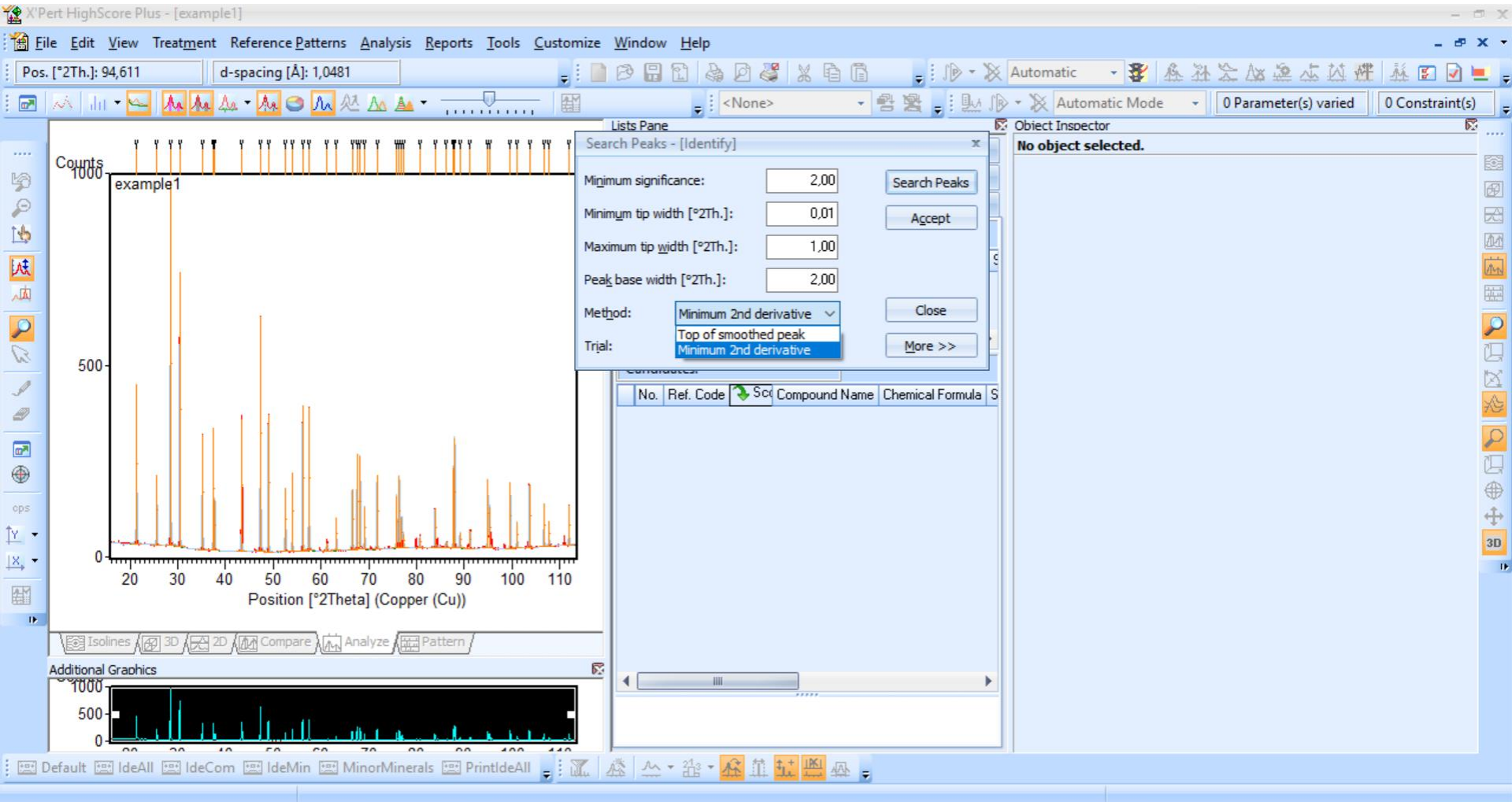
Phase identification using with HighScore(Plus)

Classical procedure : first model a bgd and then search peak



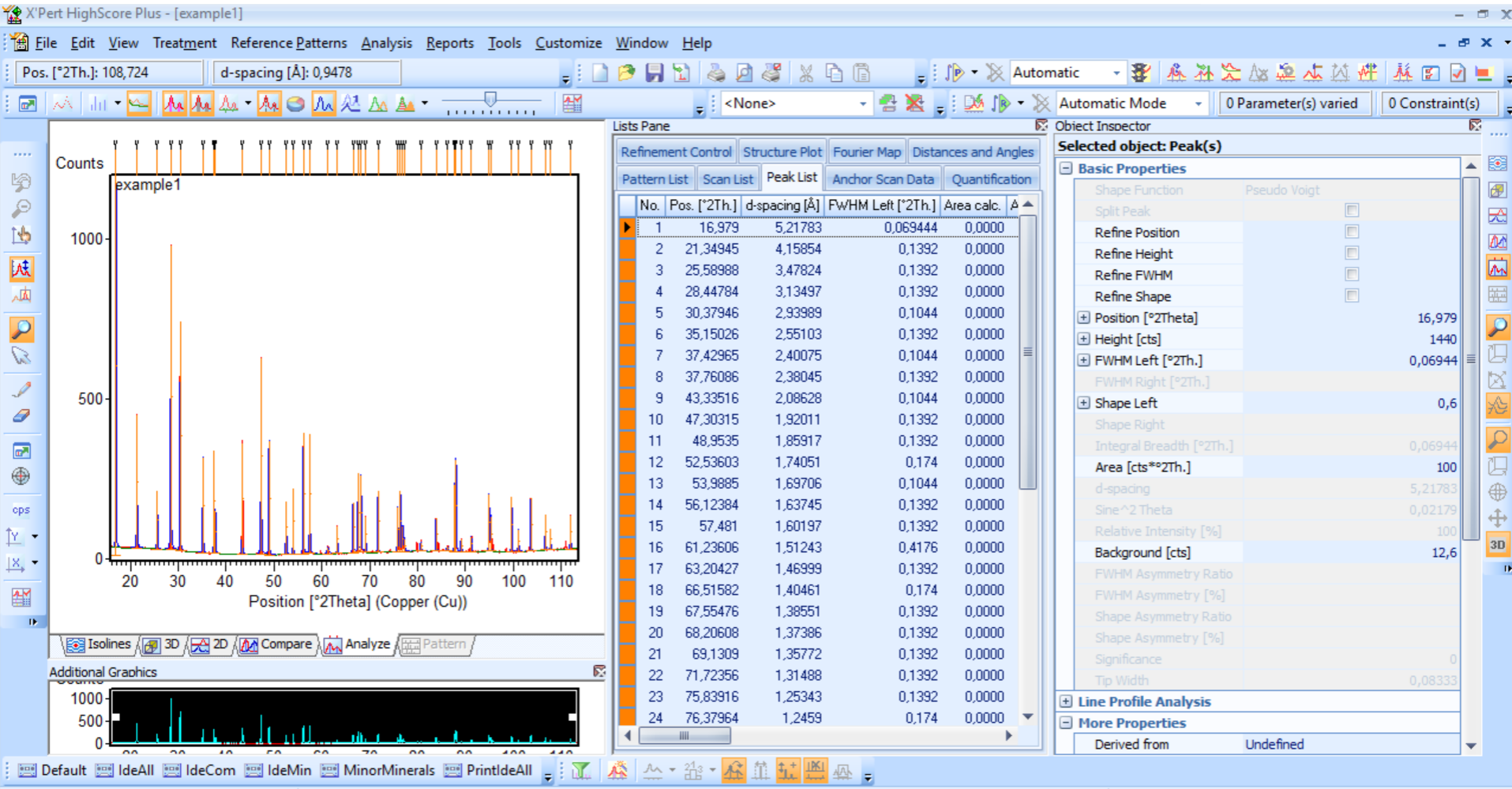
Phase identification using COD with HighScore(Plus)

Classical procedure : first model a bgd and then search peak

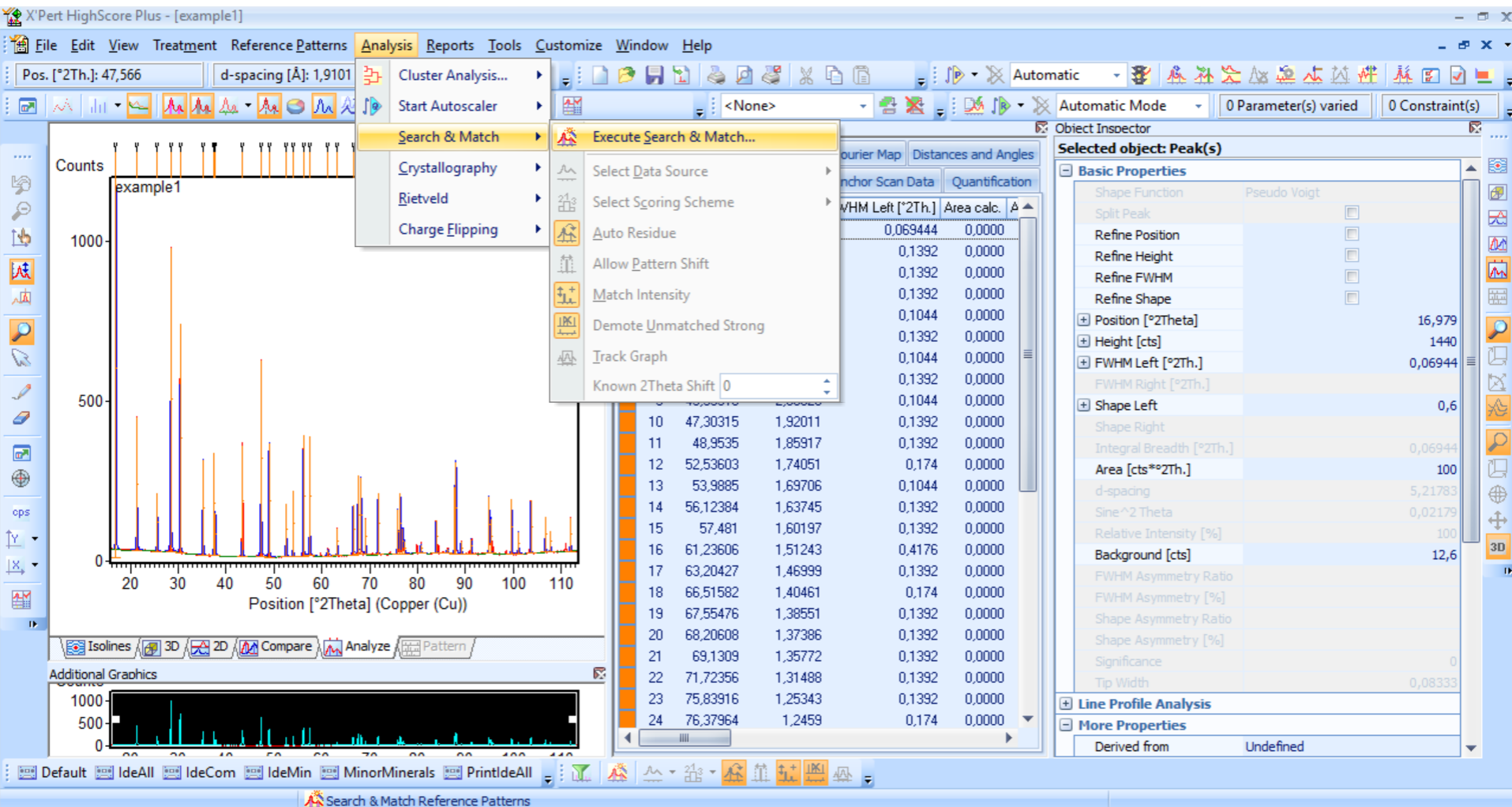


Phase identification using COD with HighScore(Plus)

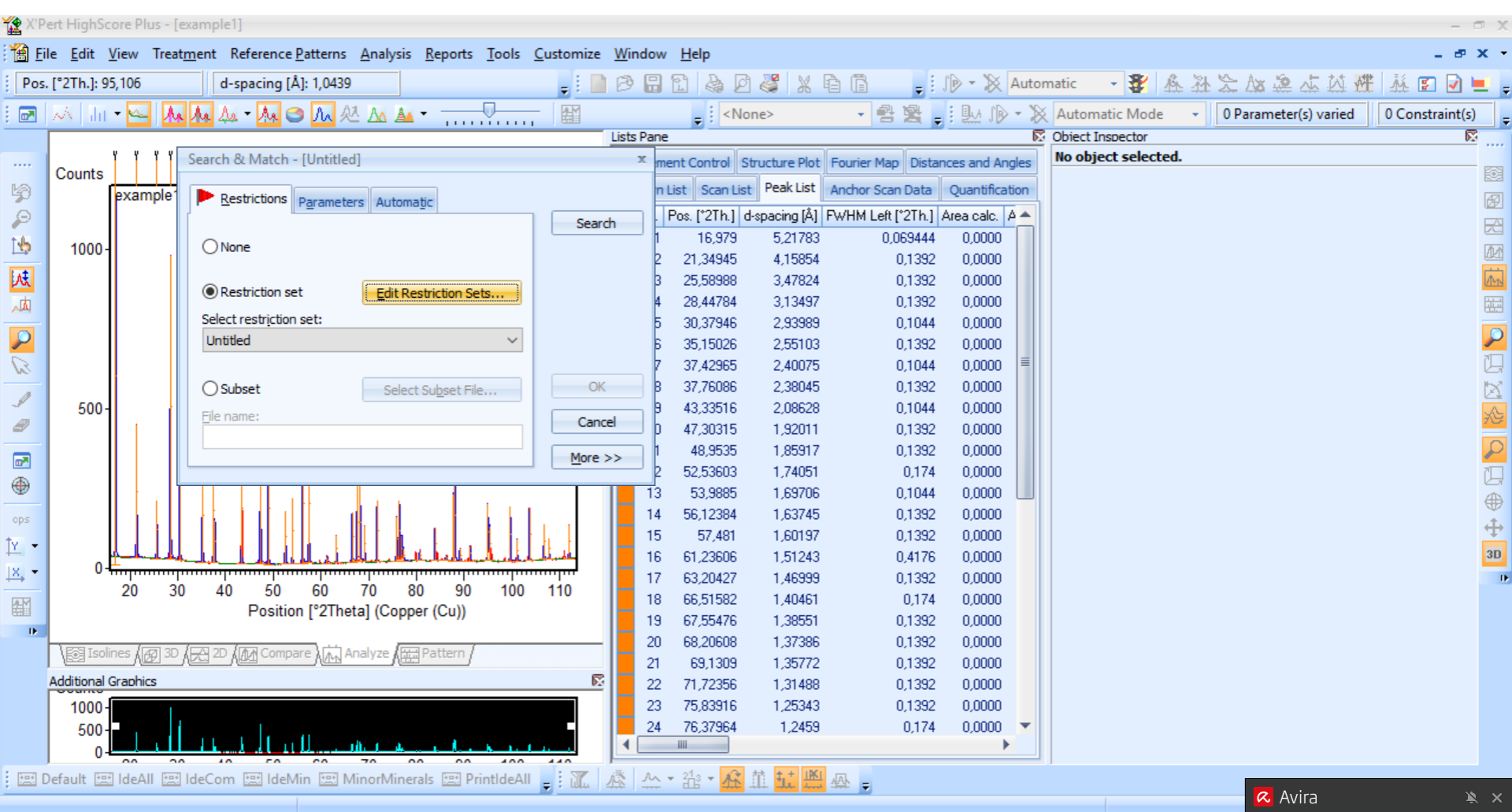
Check the peak list



Phase identification using with HighScore(Plus)

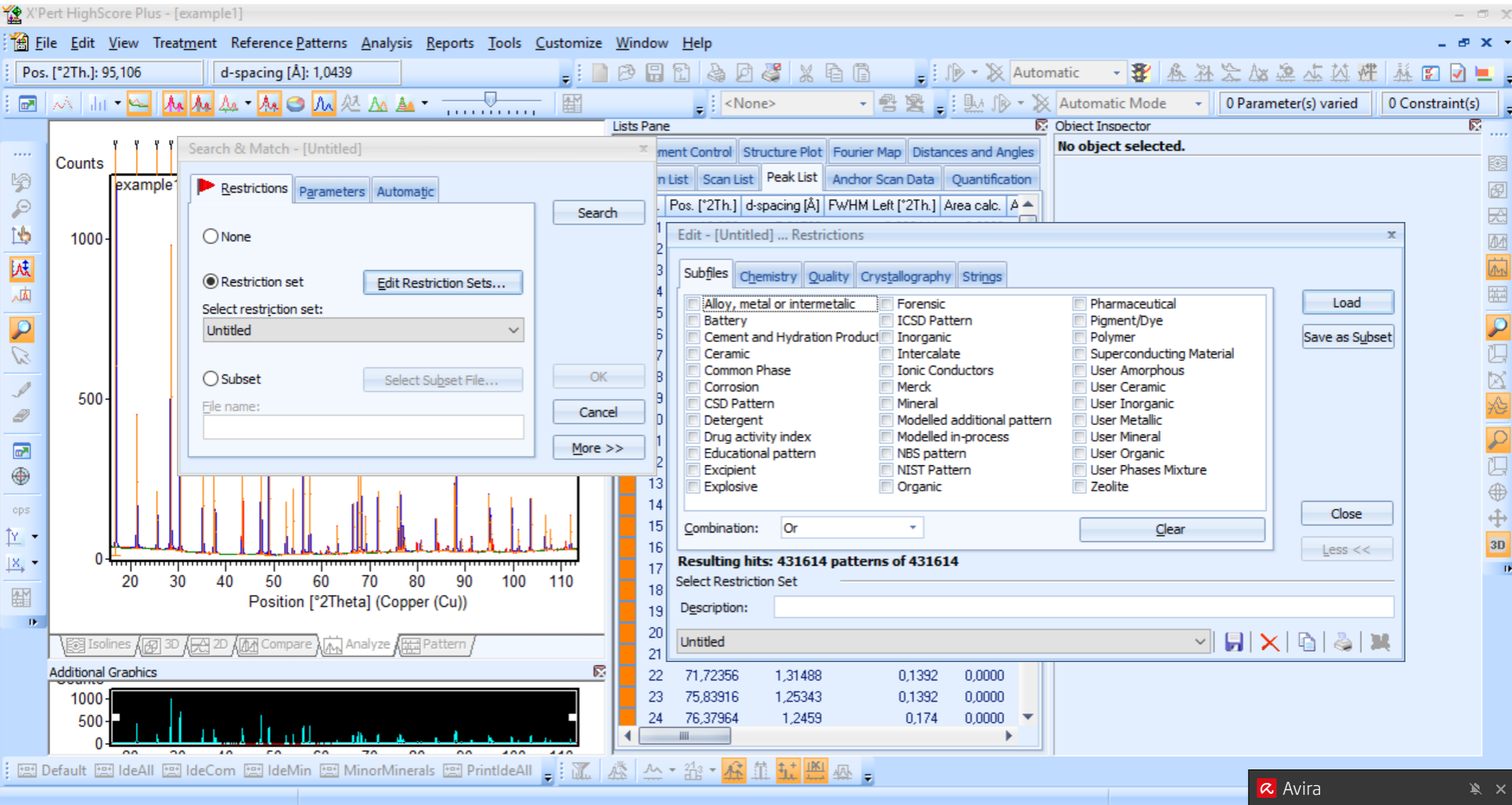


Phase identification using with HighScore(Plus)



Phase identification using with HighScore(Plus)

Search and match with restrictions



The screenshot displays the X'Pert HighScore Plus software interface. The main window shows a powder diffraction pattern with peaks labeled 'example'. The search and match process is being performed using the 'Search & Match - [Untitled]' dialog box. The 'Restrictions' tab is active, showing a list of restriction sets. The 'Restriction set' is selected, and the 'Subset' option is also visible. The 'Search' button is highlighted. The 'Edit - [Untitled] ... Restrictions' dialog box is open, showing a list of restriction sets. The 'Chemistry' tab is selected, and the 'Alloy, metal or intermetallic' restriction set is chosen. The 'Load' button is highlighted. The 'Resulting hits: 431614 patterns of 431614' are displayed. The 'Description' field is empty. The 'Untitle' restriction set is selected. The 'Load' button is highlighted. The 'Less <<' button is also visible.

Pos. [°2Th.]: 95,106 d-spacing [Å]: 1,0439

Automatic 0 Parameter(s) varied 0 Constraint(s)

Object Inspector: No object selected.

Search & Match - [Untitled]

Restrictions Parameters Automatic

None

Restriction set Edit Restriction Sets...

Select restriction set: Untitled

Subset Select Subset File...

File name:

Search

OK Cancel More >>

Edit - [Untitled] ... Restrictions

Subfiles Chemistry Quality Crystallography Strings

Alloy, metal or intermetallic Forensic Pharmaceutical

Battery ICSO Pattern Pigment/Dye

Cement and Hydration Product Inorganic Polymer

Ceramic Intercalate Superconducting Material

Common Phase Ionic Conductors User Amorphous

Corrosion Merck User Ceramic

CSD Pattern Mineral User Inorganic

Detergent Modelled additional pattern User Metallic

Drug activity index Modelled in-process User Mineral

Educational pattern NBS pattern User Organic

Excipient NIST Pattern User Phases Mixture

Explosive Organic Zeolite

Load

Save as Subset

Combination: Or Clear

Close

Less <<

Resulting hits: 431614 patterns of 431614

Select Restriction Set

Description:

Untitle

71,72356 1,31488 0,1392 0,0000

75,83916 1,25343 0,1392 0,0000

76,37964 1,2459 0,174 0,0000

Additional Graphics

Isolines 3D 2D Compare Analyze Pattern

Default IdeAll IdeCom IdeMin MinorMinerals PrintIdeAll

Avira

Phase identification using COD with HighScore(Plus)

Search and match with restrictions

Example X'Pert HighScore Plus - [example1]

Pos. [°2Th.]: 95,106 d-spacing [Å]: 1,0439

Automatic Mode 0 Parameter(s) varied 0 Constraint(s)

Search & Match - [Untitled]

Restrictions Parameters Automatic

☐ None

☒ Restriction set [Edit Restriction Sets...](#)

Select restriction set: Untitled

☐ Subset [Select Subset File...](#)

File name:

OK Cancel More >>

Search

Object Inspector: No object selected.

Edit - [Untitled] ... Restrictions

Subfiles Chemistry Quality Crystallography Strings

All of: ☒ ☒

At least one of: ☒ ☒

None of: ☒ ☒

[Periodic Table ...](#) [Clear](#) [Add Rest to None of](#)

No. of elements present

Min. Number of Elements: 0 Max. Number of Elements: 105

[Load](#) [Save as Subset](#)

Resulting hits: 431614 patterns of 431614

Select Restriction Set

Description:

Untitled

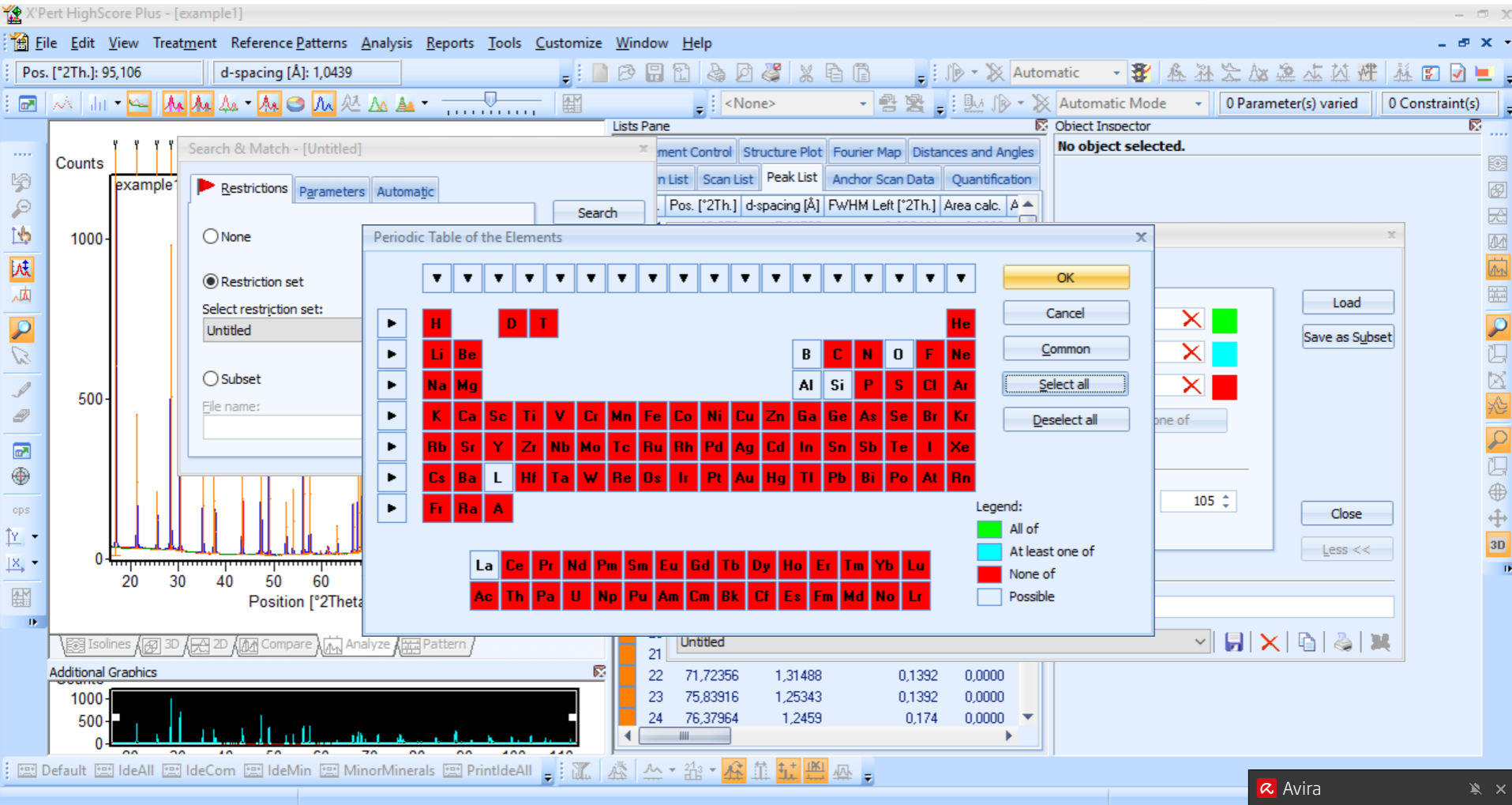
22	71,72356	1,31488	0,1392	0,0000
23	75,83916	1,25343	0,1392	0,0000
24	76,37964	1,2459	0,174	0,0000

Additional Graphics

Avira

Phase identification using with HighScore(Plus)

Search and match with restrictions



Phase identification using COD with HighScore(Plus)

Search and match with restrictions

The screenshot displays the HighScore Plus software interface. The main window shows a powder diffraction pattern with peaks labeled 'example'. The search and match window is open, showing the 'Restrictions' tab. The 'Restrictions' tab has three sub-tabs: 'Restrictions', 'Parameters', and 'Automatic'. The 'Restrictions' sub-tab is selected, showing a list of restrictions. The 'Restrictions' list is empty, and the 'Restrictions' button is highlighted. The 'Parameters' sub-tab is also visible, showing a list of parameters. The 'Automatic' sub-tab is also visible, showing a list of automatic parameters. The 'Search' button is highlighted. The 'Edit - [Untitled] ... Restrictions' window is open, showing the 'Chemistry' tab. The 'Chemistry' tab has three sub-tabs: 'Subfiles', 'Chemistry', 'Quality', 'Crystallography', and 'Strings'. The 'Chemistry' sub-tab is selected, showing a list of elements. The 'All of:' field is empty, the 'At least one of:' field is empty, and the 'None of:' field contains the elements H, He, Li, Be, C, N, F, Ne, Na, Mg, P, S, Cl, Ar, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu. The 'Periodic Table ...' button is highlighted. The 'Load' button is highlighted. The 'Save as Subset' button is highlighted. The 'Close' button is highlighted. The 'Less <<' button is highlighted. The 'Resulting hits: 1203 patterns of 431614' is displayed. The 'Select Restriction Set' dropdown is set to 'Untitled'. The 'Description:' field is empty. The table below shows the resulting hits.

Pos. [°2Th.]	d-spacing [Å]	FWHM Left [°2Th.]	Area calc. Å
71,72356	1,31488	0,1392	0,0000
75,83916	1,25343	0,1392	0,0000
76,37964	1,2459	0,174	0,0000

Phase identification using COD with HighScore(Plus)

Search and match with restrictions

The screenshot displays the HighScore Plus software interface. The main window shows a search and match results table with columns for Position, d-spacing, FWHM, and Area. The 'Search & Match - [Untitled]' dialog box is open, showing the 'Restrictions' tab. The 'Quality mark' section is highlighted with a red box, and several options are checked: Star, Indexed, Blank, Doubtful, Calculated, Modelled, Final, Rietveld, Other, Hypothetical, and Prototyping. The 'Skip marked as deleted by ICDD' option is also highlighted with a red box. The 'Resulting hits: 80 patterns of 431614' are listed in the table below.

Search & Match - [Untitled]

Restrictions Parameters Automatic

None

Restriction set

Select restriction set: Untitled

Subset

File name:

Search

OK

Cancel

More >>

Edit - [Untitled] ... Restrictions

Subfiles Chemistry Quality Crystallography Strings

Quality mark:

☐ None

☒ Star

☒ Indexed

☒ Blank

☒ Doubtful

☒ Calculated

☒ Modelled

☒ Final

☒ Rietveld

☒ Other

☒ Hypothetical

☒ Prototyping

☐ Skip marked as deleted by ICDD

☐ Skip no RIR value

☐ Skip non-ambient temperature

☐ Skip non-ambient pressure

☐ Skip alternate patterns

☐ Skip patterns without reference scan

Clear

Load

Save as Subset

Close

Less <<

Resulting hits: 80 patterns of 431614

Select Restriction Set

Description:

Untitled

Pos. [°2Th.]	d-spacing [Å]	FWHM Left [°2Th.]	Area calc. Å
22	71,72356	1,31488	0,1392 0,0000
23	75,83916	1,25343	0,1392 0,0000
24	76,37964	1,2459	0,174 0,0000

Phase identification using with HighScore(Plus)

Search and match with restrictions

Example X'Pert HighScore Plus - [example1]

Pos. [°2Th.]: 95,106 d-spacing [Å]: 1,0439

Automatic Mode 0 Parameter(s) varied 0 Constraint(s)

Search & Match - [Untitled]

Restrictions Parameters Automatic

☐ None

☒ Restriction set [Edit Restriction Sets...](#)

Select restriction set: Untitled

☐ Subset [Select Subset File...](#)

File name:

OK Cancel More >>

Search

Counts

example

Position [°2Theta] (Copper (Cu))

Additional Graphics

Isolines 3D 2D Compare Analyze Pattern

Object Inspector No object selected.

Element Control Structure Plot Fourier Map Distances and Angles

Scan List Peak List Anchor Scan Data Quantification

Pos. [°2Th.] d-spacing [Å] FWHM Left [°2Th.] Area calc. Å

Edit - [Untitled] ... Restrictions

Subfiles Chemistry Quality Crystallography Strings

Min Max

a [Å]:

b [Å]:

c [Å]:

alpha [°]:

beta [°]:

gamma [°]:

ratio a/c:

Density [g/cm**3]:

No. of Formula Units (Z):

Reference Intensity Ratio:

Cell Volume [Å**3]:

Space Group Number:

Crystal System:

Clear

Load Save as Subset

Min - Max Value - Deviation [%]

Resulting hits: 80 patterns of 431614

Select Restriction Set

Description:

Untitled

	Min	Max		Min	Max
a [Å]:			Density [g/cm**3]:		
b [Å]:			No. of Formula Units (Z):		
c [Å]:			Reference Intensity Ratio:		
alpha [°]:			Cell Volume [Å**3]:		
beta [°]:			Space Group Number:		
gamma [°]:			Crystal System:		
ratio a/c:					

22 71,72356 1,31488 0,1392 0,0000

23 75,83916 1,25343 0,1392 0,0000

24 76,37964 1,2459 0,174 0,0000

Avira

Phase identification using COD with HighScore(Plus)

Search and match with restrictions

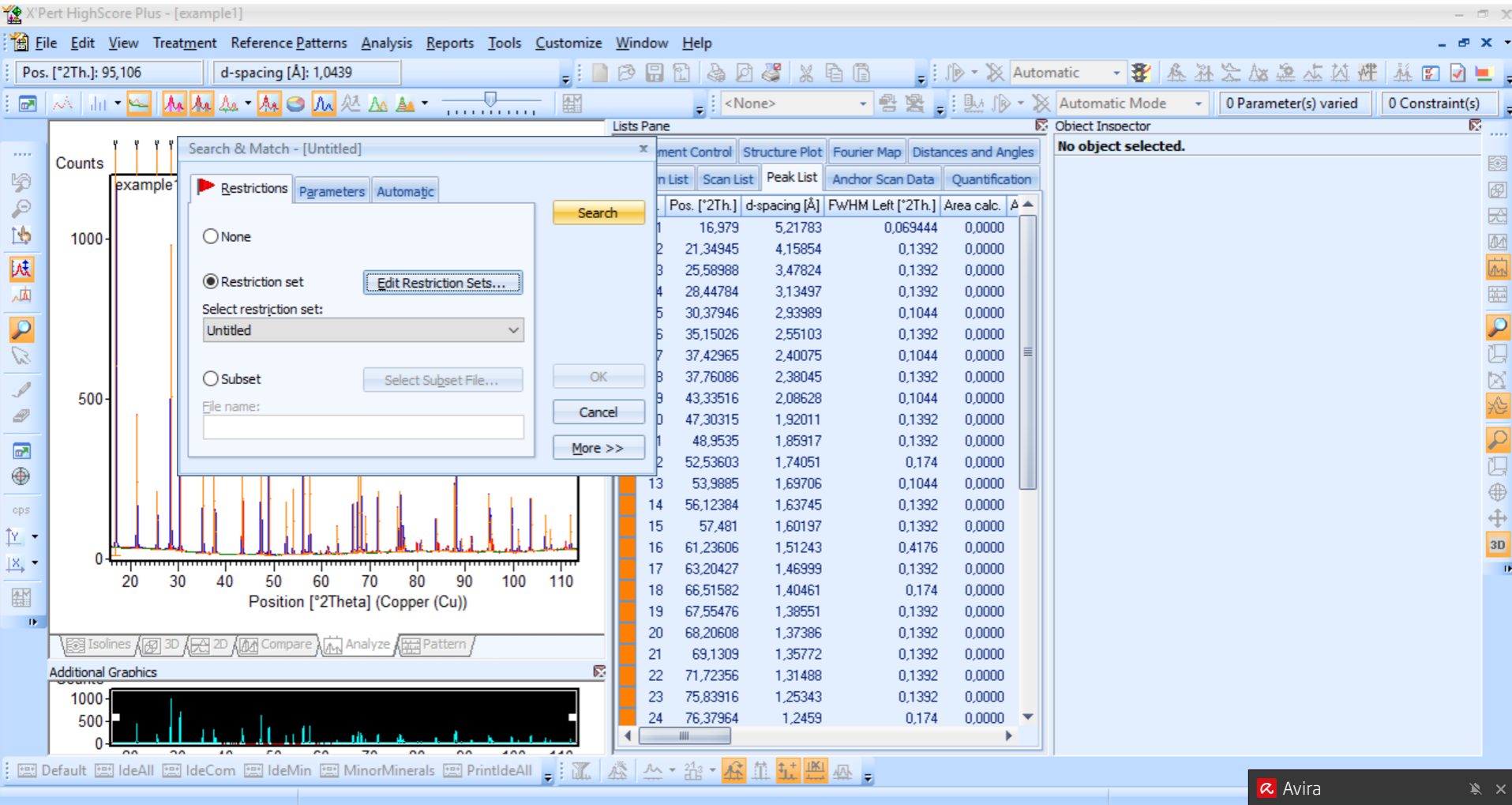
The screenshot displays the X'Pert HighScore Plus software interface. The main window shows a powder diffraction pattern with peaks labeled 'example'. The search and match process is being performed using the 'Search & Match - [Untitled]' dialog box. The 'Restrictions' tab is active, showing options for 'None', 'Restriction set' (selected), and 'Subset'. The 'Restriction set' option is further configured with 'Untitled' as the selected set. The 'Edit - [Untitled] ... Restrictions' dialog box is also open, showing fields for 'Compound Name', 'Mineral Name', 'Formula', 'Color', 'Author', and 'Journal', all of which are currently empty. The 'Exact Match' checkbox is checked. The 'Load' button is visible. Below the search dialog, the 'Resulting hits: 80 patterns of 431614' are listed. The 'Select Restriction Set' dropdown is set to 'Untitled'. The 'Description' field is empty. The 'List Pane' on the right shows a table of search results.

Pos. [°2Th.]	d-spacing [Å]	FWHM Left [°2Th.]	Area calc. Å
71,72356	1,31488	0,1392	0,0000
75,83916	1,25343	0,1392	0,0000
76,37964	1,2459	0,174	0,0000

Additional Graphics: A small inset window shows a zoomed-in view of the diffraction pattern peaks.

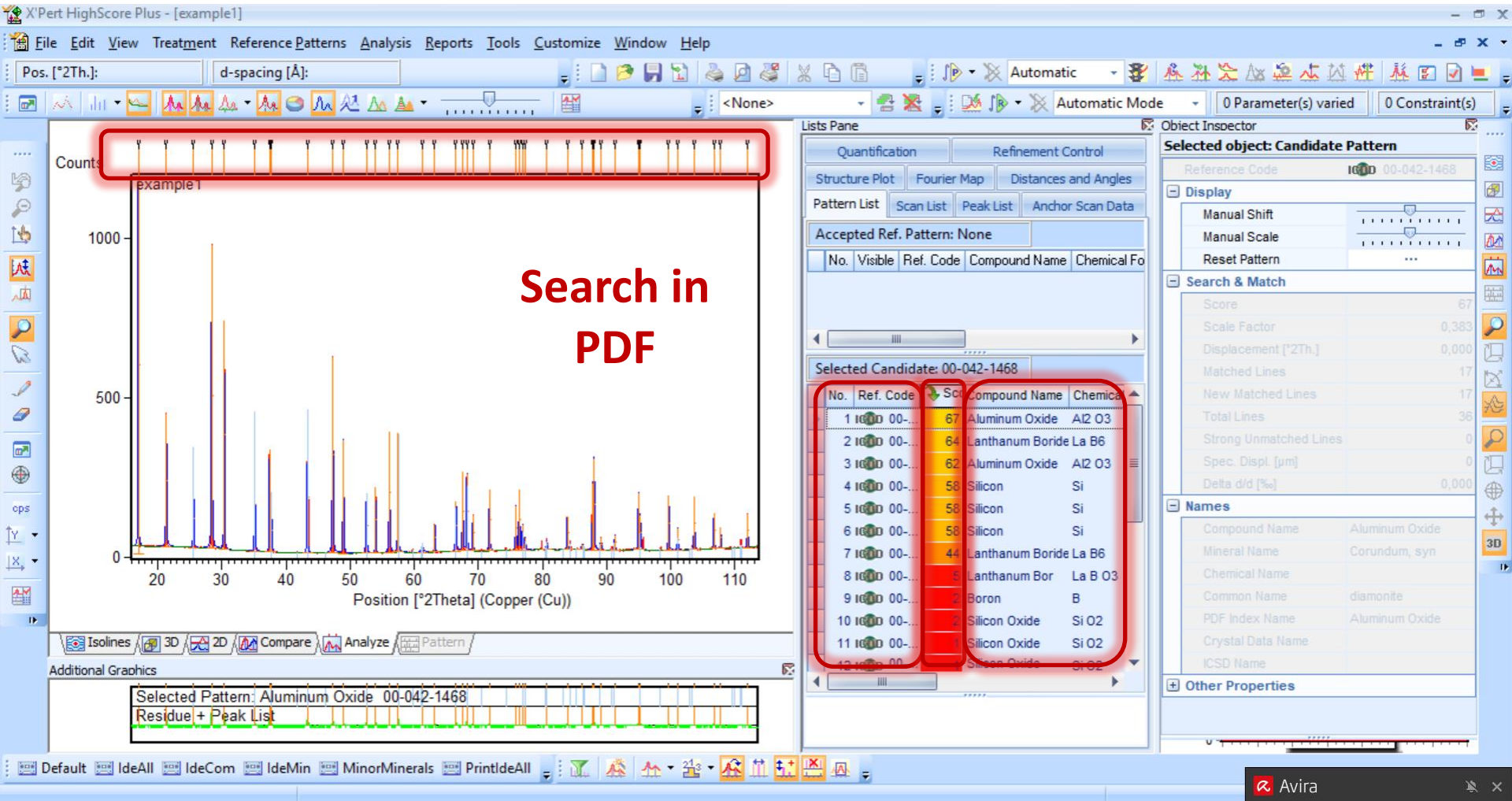
Phase identification using COD with HighScore(Plus)

Search and match with restrictions



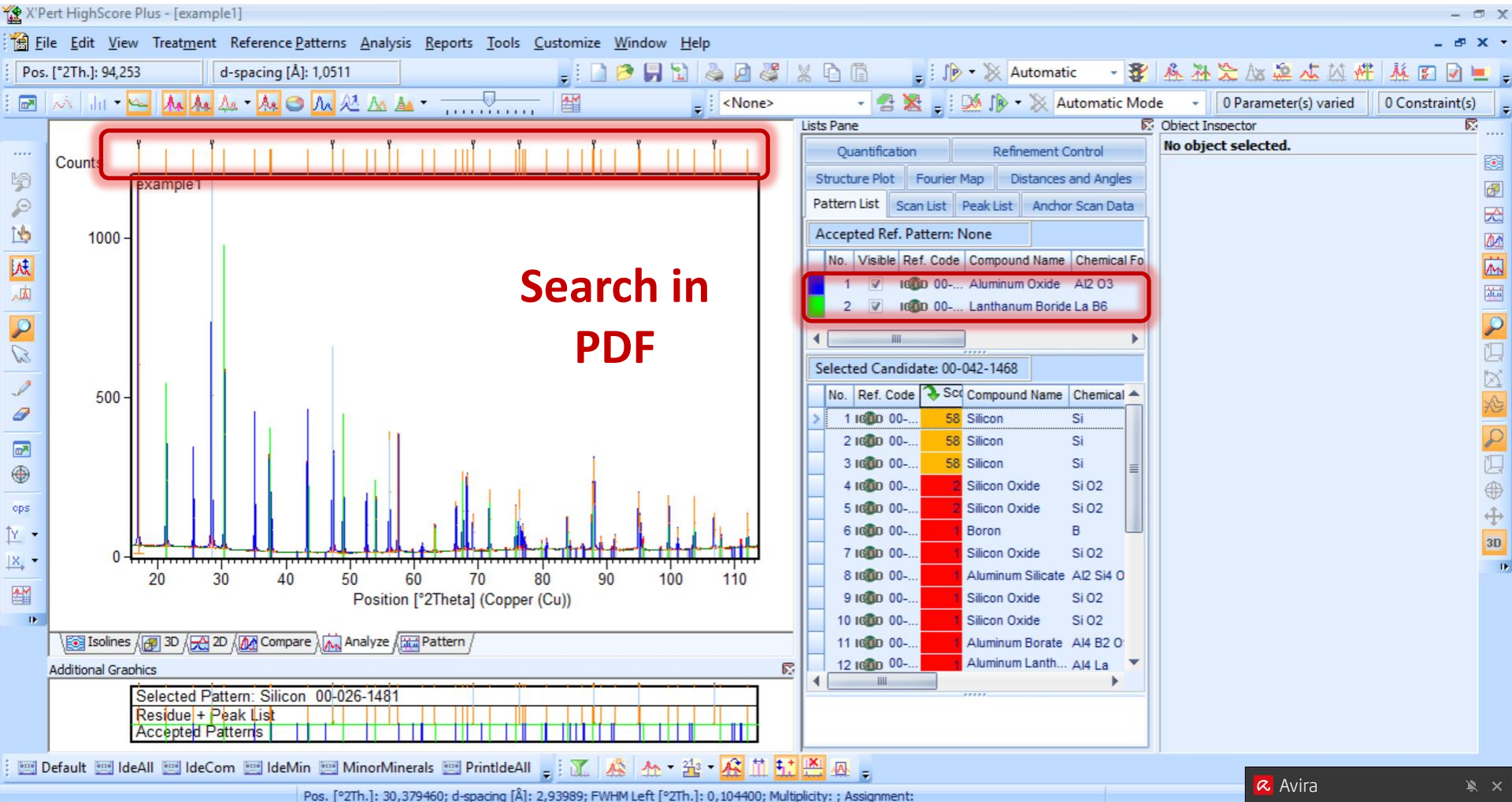
Phase identification using COD with HighScore(Plus)

Search and match with restrictions



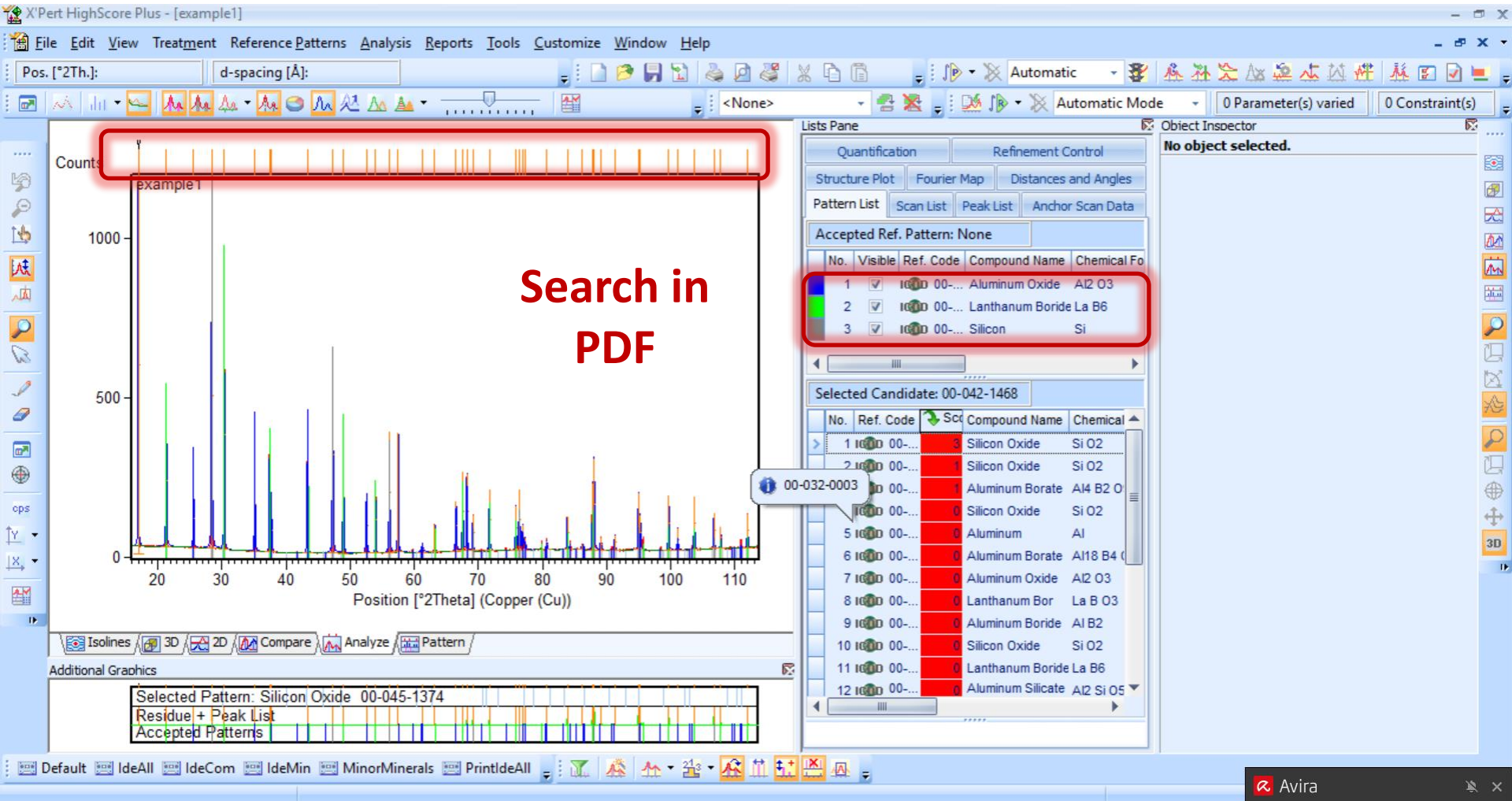
Phase identification using COD with HighScore(Plus)

Search and match with restrictions

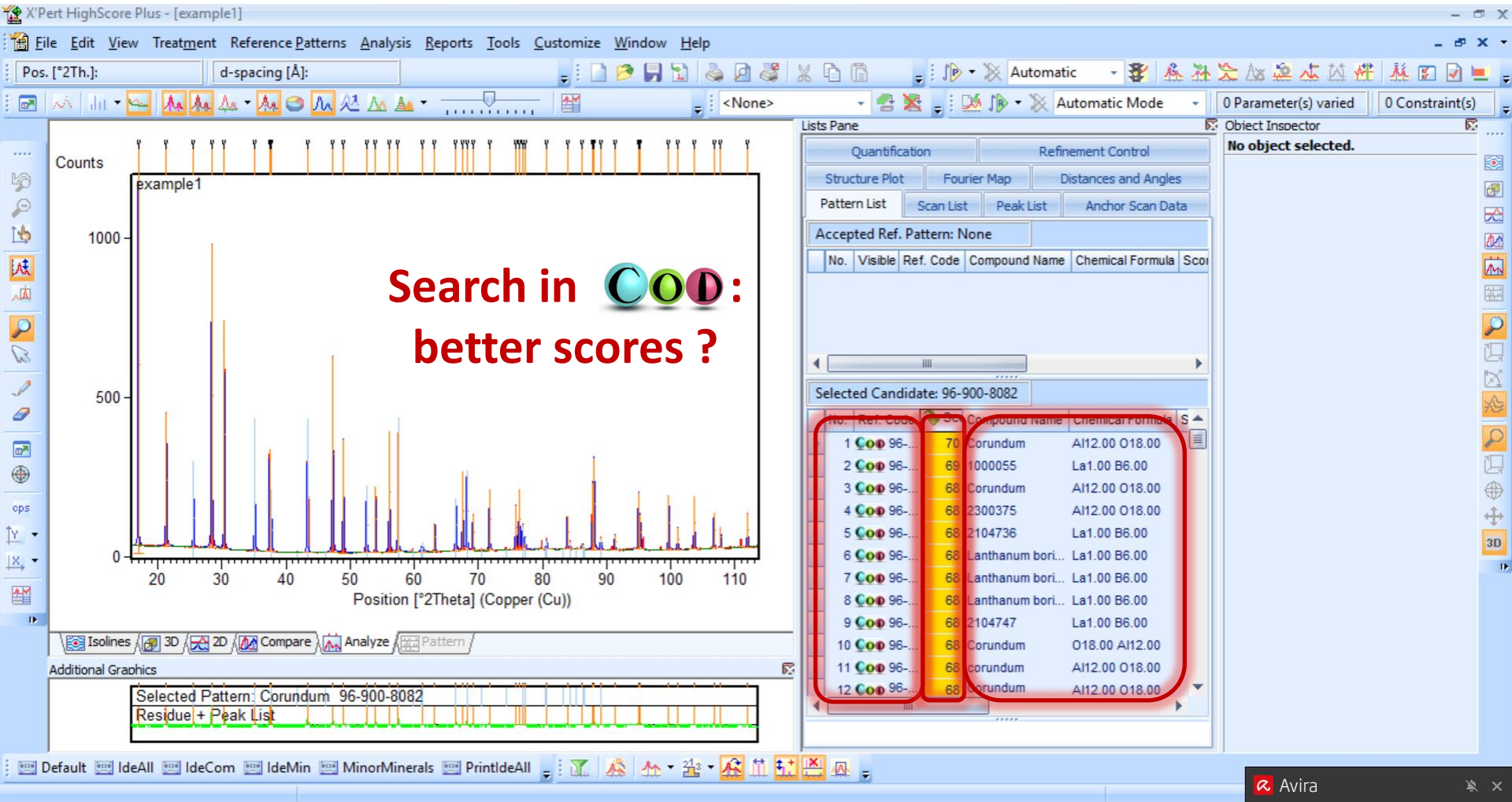


Phase identification using with HighScore(Plus)

Search and match with restrictions



Phase identification using with HighScore(Plus)



Phase identification using COD with HighScore(Plus)

COD reference patterns are accessible as well as PDF ones

X'Pert HighScore Plus - [example1]

Pos. [°2Th.]: 72,514 d-spacing [Å]: 1,3025 Automatic

Reference Pattern: 96-900-8082

Counts

example1

Name and formula

Reference code: 96-900-8082

Mineral name: Corundum

Compound name: Corundum

Common name: Corundum

Chemical formula: $\text{Al}_{12.00}\text{O}_{18.00}$

Crystallographic parameters

Crystal system: Hexagonal

Space group: R -3 c

Space group number: 167

a (Å): 4,7590

b (Å): 4,7590

c (Å): 12,9910

Alpha (°): 90,0000

Beta (°): 90,0000

Gamma (°): 120,0000

Calculated density (g/cm³): 3,99

Volume of cell (10⁶ pm³): 254,80

RIR: 1,00

Additional Graphics

Isolines 3D 2D Co

Selected Pattern: Corundum

Residue + Peak List

Save As... Copy Print Graphics... Print All... Intensity Scale Angle Scale Wavelength 1,54060 Close

Parameter(s) varied: 0 Constraint(s)

Object Inspector

Selected object: Candidate Pattern

Reference Code: COD 96-900-8082

Display

Manual Shift Manual Scale Reset Pattern

Search & Match

Score	70
Scale Factor	0,360
Displacement [°2Th.]	0,000
Matched Lines	14
New Matched Lines	14
Total Lines	25
Strong Unmatched Lines	0
Spec. Displ. (μm)	0
Delta d/d [%]	0,000

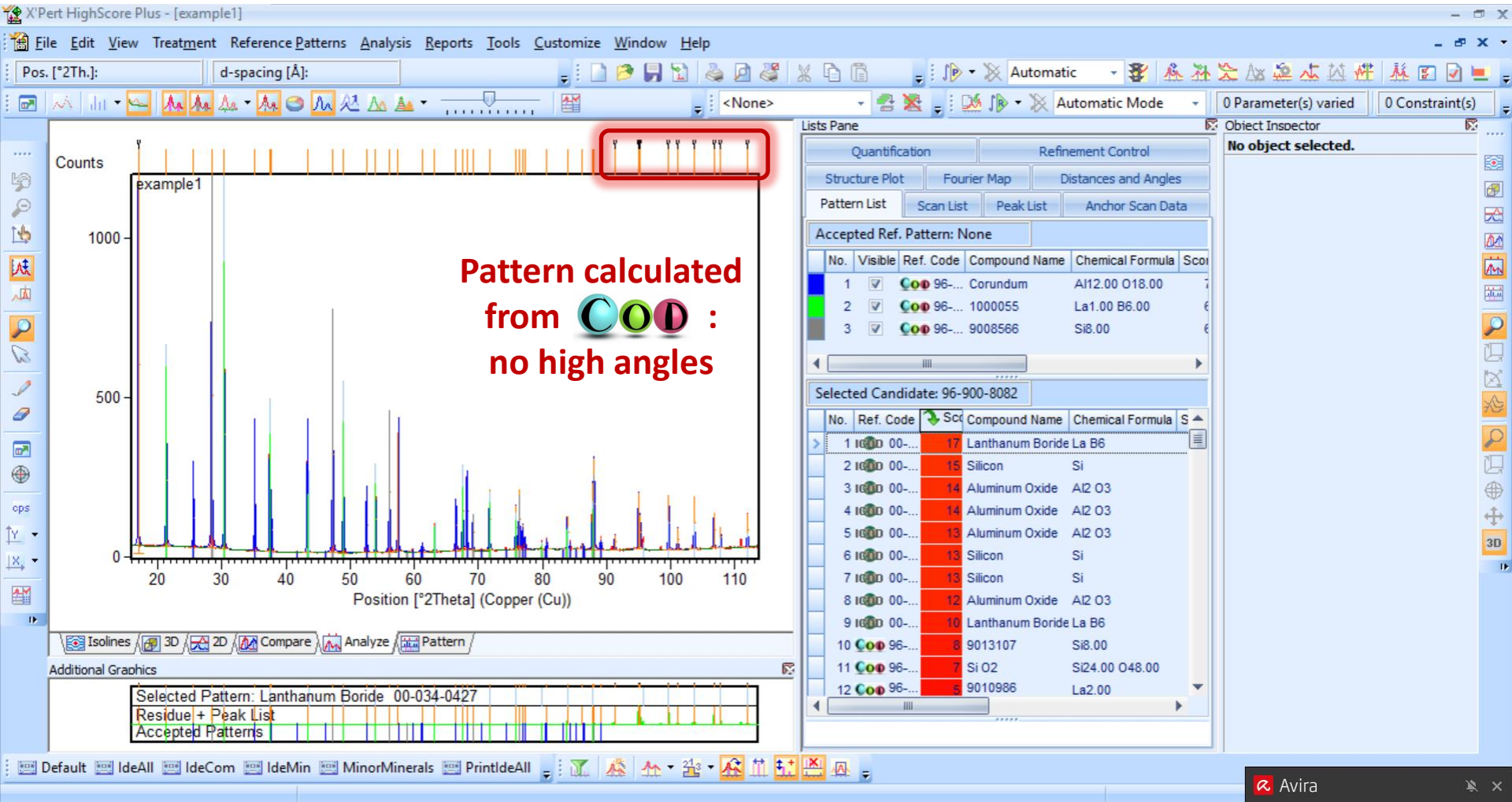
Names

Compound Name	Corundum
Mineral Name	Corundum
Chemical Name	
Common Name	Corundum
PDF Index Name	
Crystal Data Name	
ICSD Name	

Other Properties

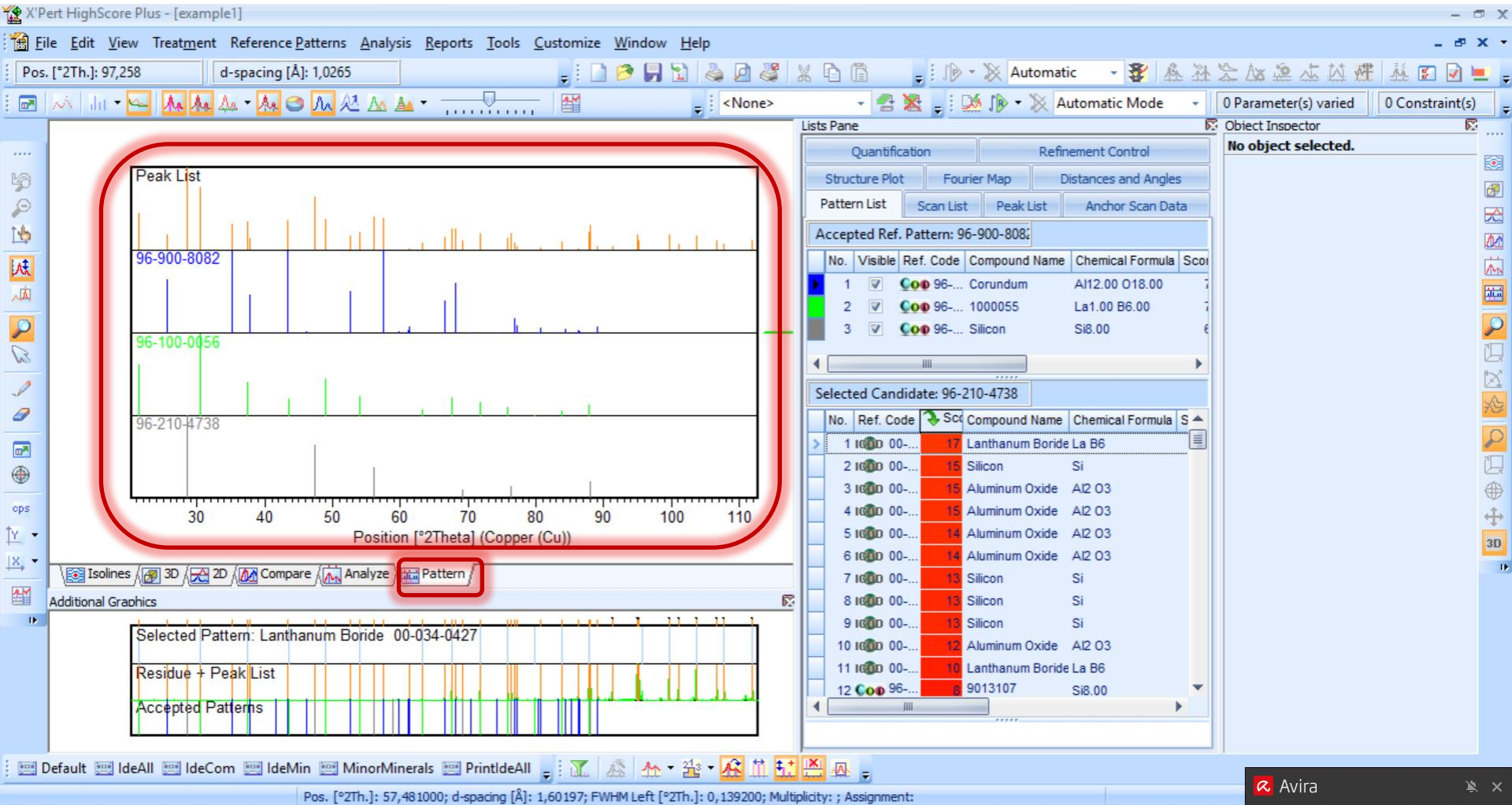
Avira

Phase identification using COD with HighScore(Plus)



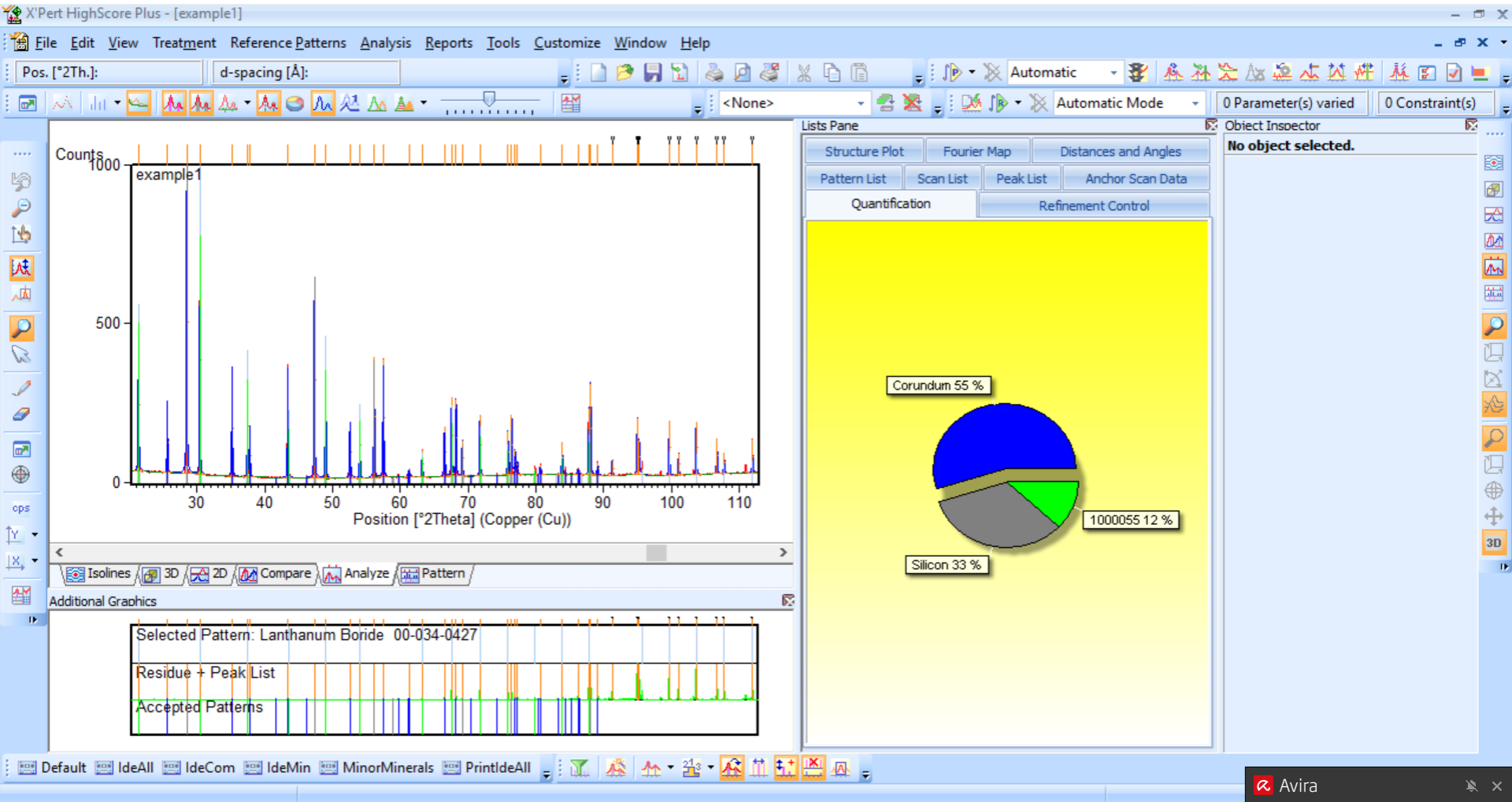
Phase identification using COD with HighScore(Plus)

Visualisation options...



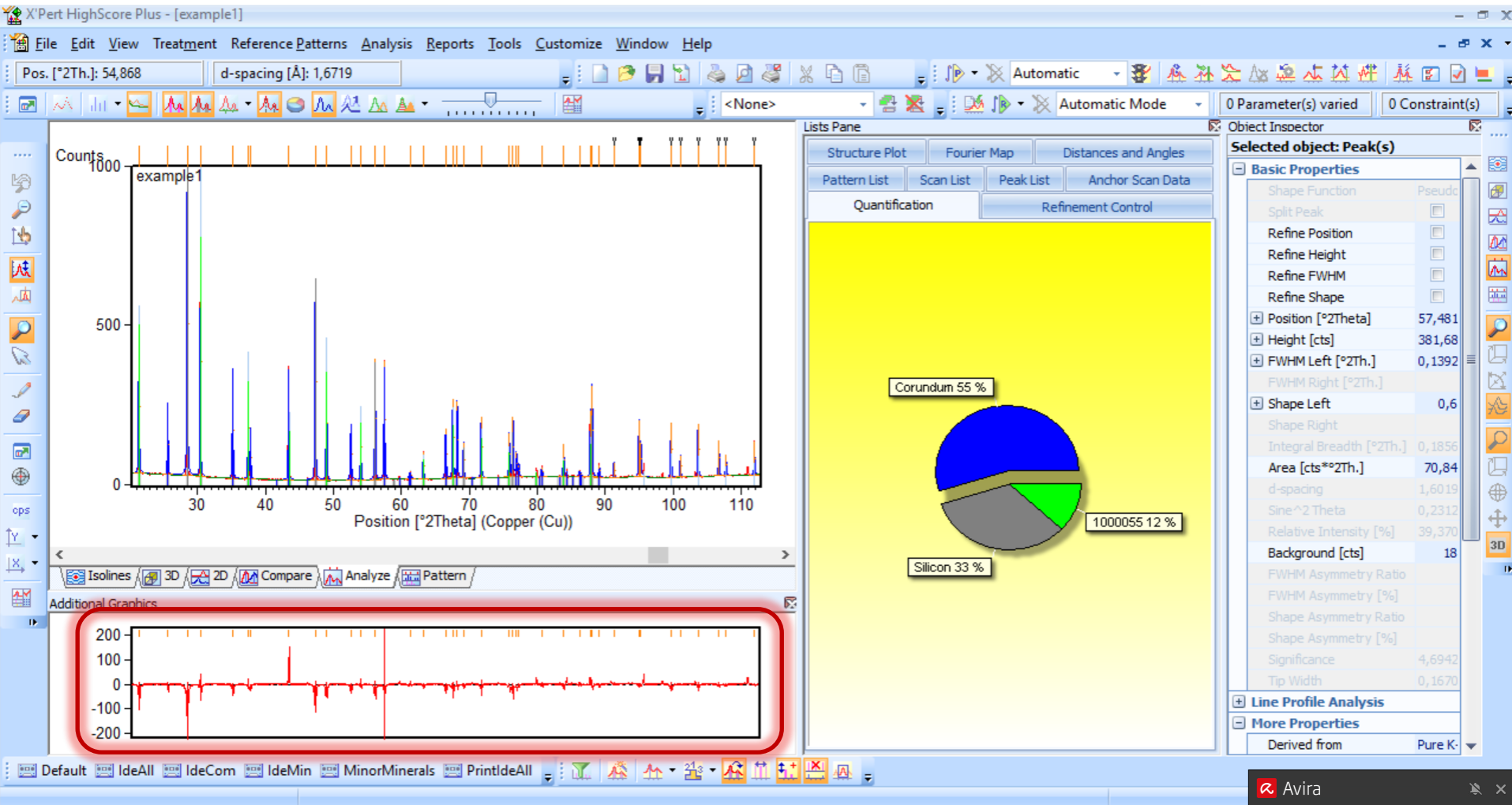
Phase identification using COD with HighScore(Plus)

« semi quantitative » analysis from RIR



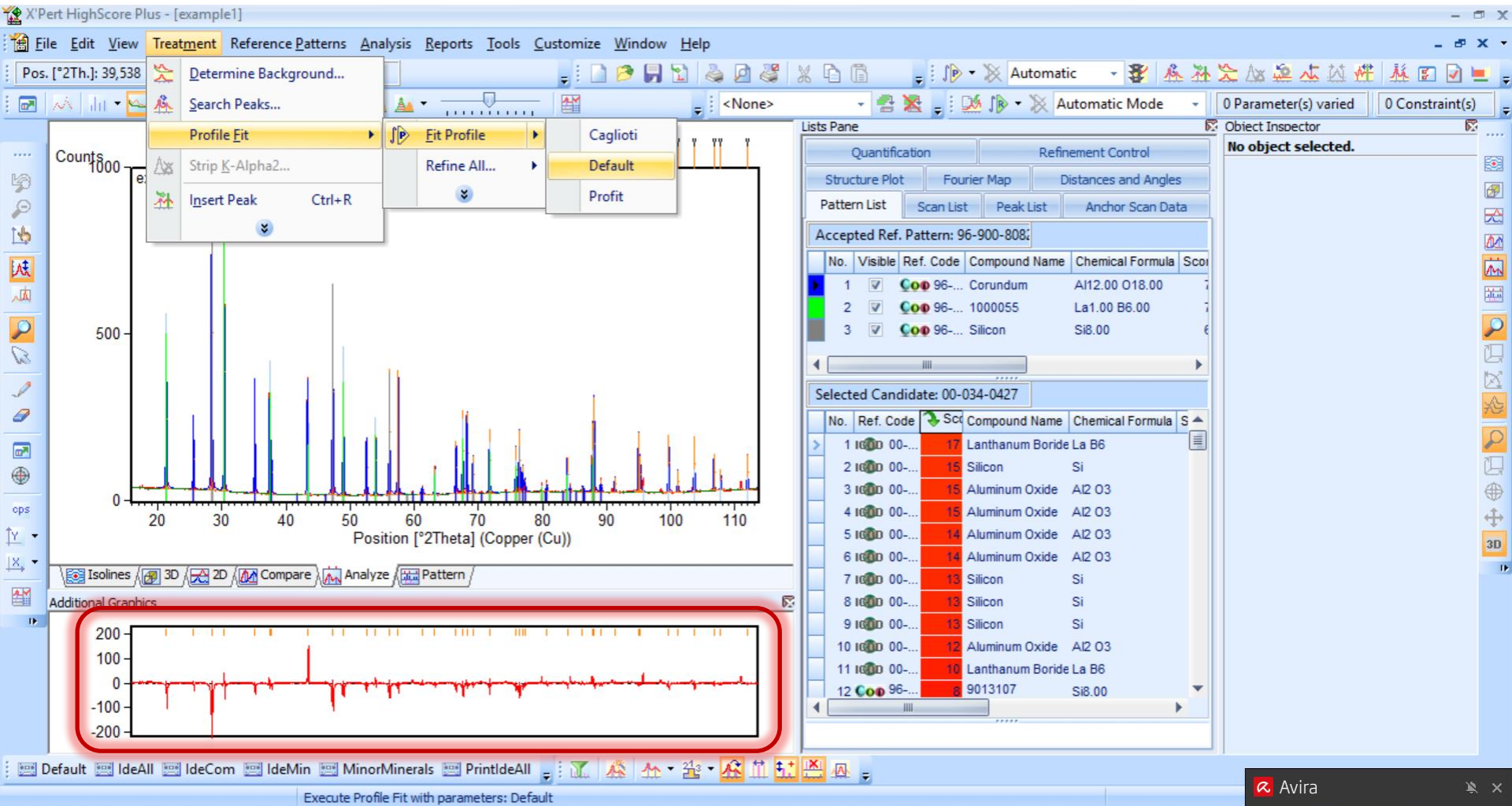
Phase identification using with HighScore(Plus)

« semi quantitative » analysis from RIR without refinement



Phase identification using COD with HighScore(Plus)

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



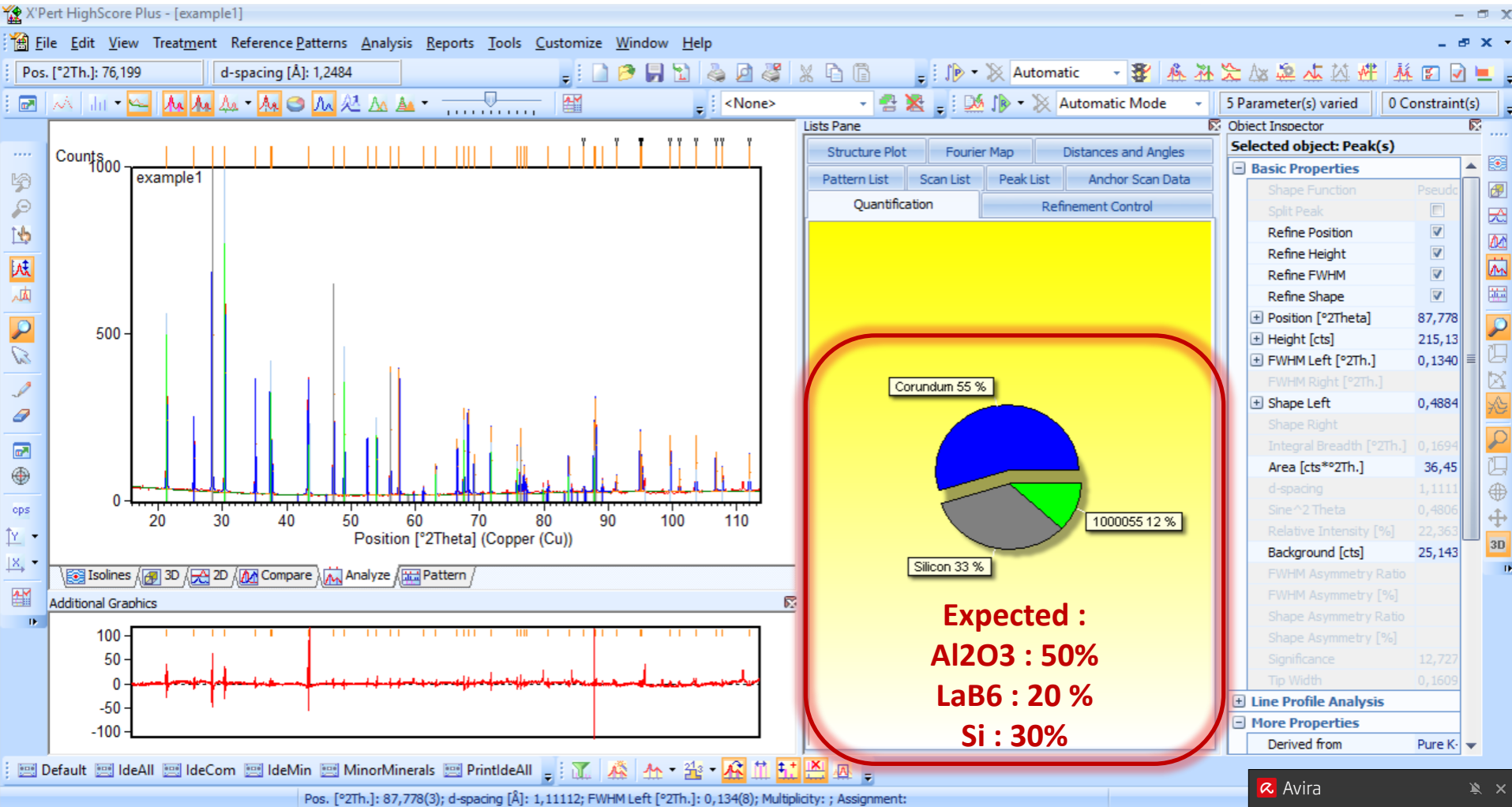
Phase identification using COD with HighScore(Plus)

« 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



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](#)
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 - [Documentation](#)
- [SunBim](#)
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Phase identification using



with QualX

Software IC

Institute of Crystallography - CNR - Bari

Contact IC CNR

Software Available

The software packages currently developed at IC are:

- [Shelx](#): 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 MILKONE.
- [IL MILKONE](#): a suite of computer programs devoted to protein crystal structure determination by X-ray crystallography. The package currently contains the program SHIRAS, for the solution and refinement of small structures.
- [EXPlore](#): 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.
- [Quant](#): a Rietveld program for quantitative phase analysis of polycrystalline mixtures from powder diffraction data.
- [Imaging](#): a suite of programs for the supra- and sub-molecular X-ray imaging of nanoscale materials with SAXS, WAXS, GISAXS and GPCWAXS techniques.

- [Shelx](#)
 - [Download](#)
- [IL MILKONE](#)
 - [Download](#)
- [EXPlore](#)
 - [Download](#)
 - [Documentation](#)
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Phase identification using with QualX

QualX2 download

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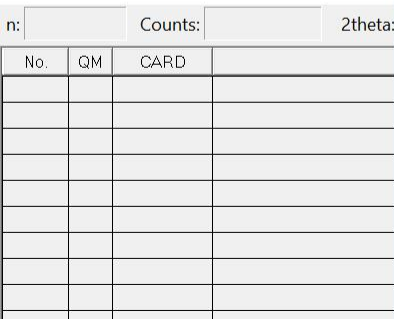
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- **QualX2**: a computer program for phase identification using powder diffraction data.

- **Quantx**: a Win95 program for quantitative phase analysis of polycrystalline mixtures from powder diffraction data.
- **Imaging**: a suite of programs for the supra- and sub-molecular X-ray imaging of nanoscale materials with SAXS, WAXS, GPC-SAXS and GPC-WAXS techniques.

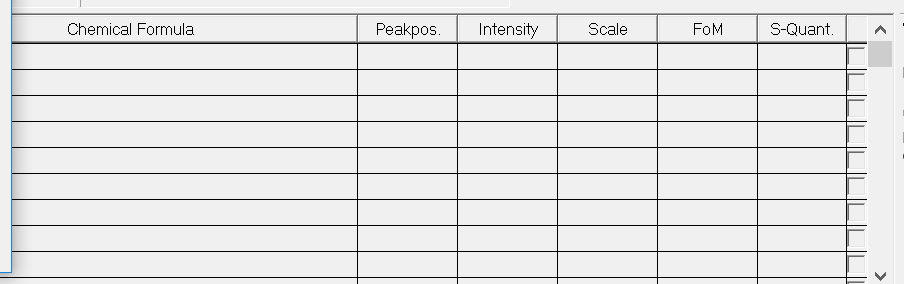
—



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.

Multiple readable files

—



—



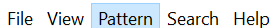
QualX - [C:\Program Files\QualX\examples\example1.dat]

File View Pattern Search Help

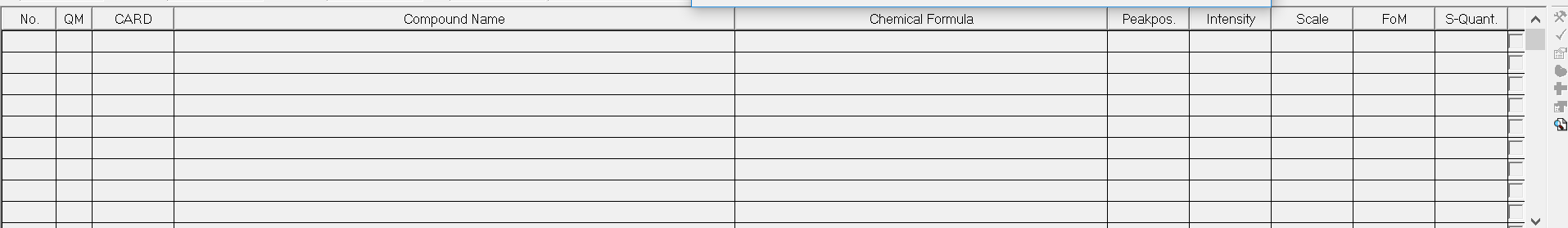


with QualX

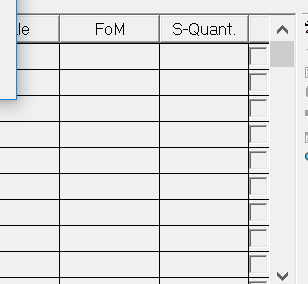
—



Very intuitive handling to model bgd and find peaks



Very intuitive handling to model bgd and find peaks

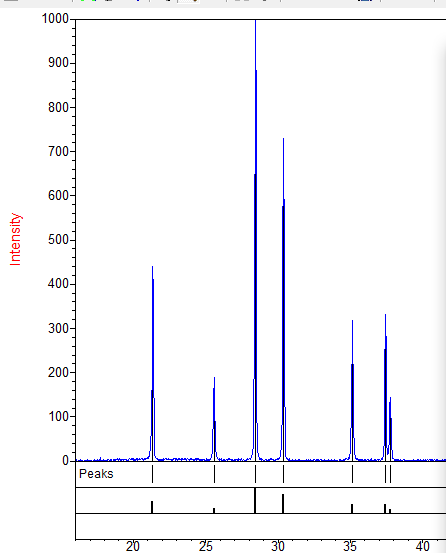


Search in COD or PDF database



Search restrictions

Exp. peaks



n:	466	Counts:	1007.38	2theta:	29
----	-----	---------	---------	---------	----

[illegible]


Restraints
✕

Composition

Subfiles

Chemical name

Entries

Symmetry

Cell and properties

IA

IIA

IIIB

IVB

VB

VIB

VIIb

VIIIb

IB

IIB

IIIA

IVA

VA

VIA

VIIA

VIII

Period 1

1 H

2 He

Period 2

3 Li

4 Be

5 B

6 C

7 N

8 O

9 F

10 Ne

Period 3

11 Na

12 Mg

13 Al

14 Si

15 P

16 S

17 Cl

18 Ar

Period 4

19 K

20 Ca

21 Sc

22 Ti

23 V

24 Cr

25 Mn

26 Fe

27 Co

28 Ni

29 Cu

30 Zn

31 Ga

32 Ge

33 As

34 Se

35 Br

36 Kr

Period 5

37 Rb

38 Sr

39 Y

40 Zr

41 Nb

42 Mo

43 Tc

44 Ru

45 Rh

46 Pd

47 Ag

48 Cd

49 In

50 Sn

51 Sb

52 Te

53 I

54 Xe

Period 6

55 Cs

56 Ba

57 La

58 Ce

59 Pr

60 Nd

61 Pm

62 Sm

63 Eu

64 Gd

65 Tb

66 Dy

67 Ho

68 Er

69 Tm

70 Yb

71 Lu

Period 7

87 Fr

88 Ra

89 Ac

90 Th

91 Pa

92 U

93 Np

94 Pu

95 Am

96 Cm

97 Bk

98 Cf

99 Es

100 Fm

101 Md

102 No

103 Lr

LN

AC

Si AND Al AND O AND B AND La

☒ And
 ☐ Or
 ☐ Not
 ☐ Only
 ☐ Just

Clear

of elements: -

min. max.

Load cards

Load and Merge Cards

Search with restraints

Cancel all restraints!

Close

Help

Exp-2th	Exp-1
21.344	439.56
25.578	188.43
28.449	1000.00
30.392	730.19
35.148	317.22
37.439	331.93
37.758	143.25
43.355	373.79
47.299	646.46
48.952	376.67
52.548	173.73
53.998	214.02
56.115	398.56
57.478	395.37
61.306	31.53
63.191	91.08
66.526	167.19
67.541	261.21
68.208	259.62

[illegible]

Phase identification using COD with QualX

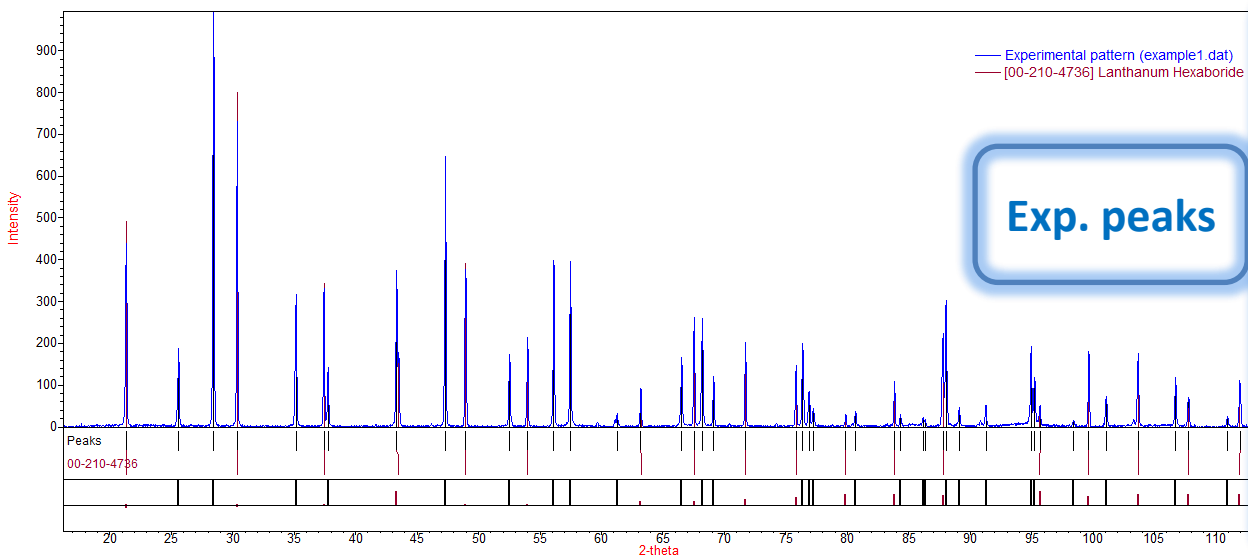


Found results

phase
1

QualX - [C:\Program Files\QualX\examples\example1.dat]

File View Pattern Search Help



Exp-2th	Exp-I	2104736	2104736
21.34	439.6	21.36	492.4
25.58	188.4		
28.45	1000.0		
30.39	730.2	30.38	799.3
35.15	317.2		
37.44	331.9	37.44	342.3
37.76	143.3		
43.35	373.8	43.50	174.8
47.30	646.5		
48.95	376.7	48.95	391.0
52.55	173.7		
54.00	214.0	53.99	208.1
56.11	398.6		
57.48	395.4		
61.31	31.5		
63.19	91.1	63.22	79.0
66.53	167.2		
67.54	261.2	67.54	225.7
68.21	259.6		

n: 3185 Counts: -299.90 2theta: 108.321 d: 0.950 Estimation of background

No.	QM	ICRD	Compound Name	Chemical Formula	Peakpos.	Intensity	Scale	PoM	S Quant.
1	C	00-210-4736	Lanthanum Hexaboride	B6 La	0.93211	0.73330	0.79926	0.83281	10.681
2	C	00-210-4748	Silicon [Silicon]	Si	0.97081	0.86807	1.0041	0.81938	4.868
3	C	00-110-1023	Lanthanum boride (1/6)	La B6	0.93370	0.63849	0.80784	0.81394	10.190
4	C	00-410-4917		Si	0.97127	0.79532	1.0302	0.80498	4.738
5	C	00-900-7496	[Corundum]	Al2 O3	0.79487	0.77333	0.37634	0.78305	1.097
6	C	00-230-0375		Al2 O3	0.80006	0.76722	0.37686	0.77537	1.089
7	C	00-100-8993	Europium boride carbide (1/5.8/0.2)	Eu B5.8 C0.2	0.72895	0.63809	0.80325	0.77079	12.564
8	C	00-100-8907	Europium boride carbide (1/5.8/0.2)	Eu (B5.8 C0.2)	0.72895	0.63809	0.80325	0.77079	12.564
9	C	00-230-0448	aluminium oxide [corundum]	Al2 O3	0.78197	0.77795	0.37457	0.76188	1.093
10	C	00-152-1500	Ba16O667O24W622O220	Ba16O667O24W622O220	0.00000	0.00000	0.78507	0.75000	0.000

Matched POW_COD C 234 Selected Card 00-210-4736 Lanthanum Hexaboride B6 La

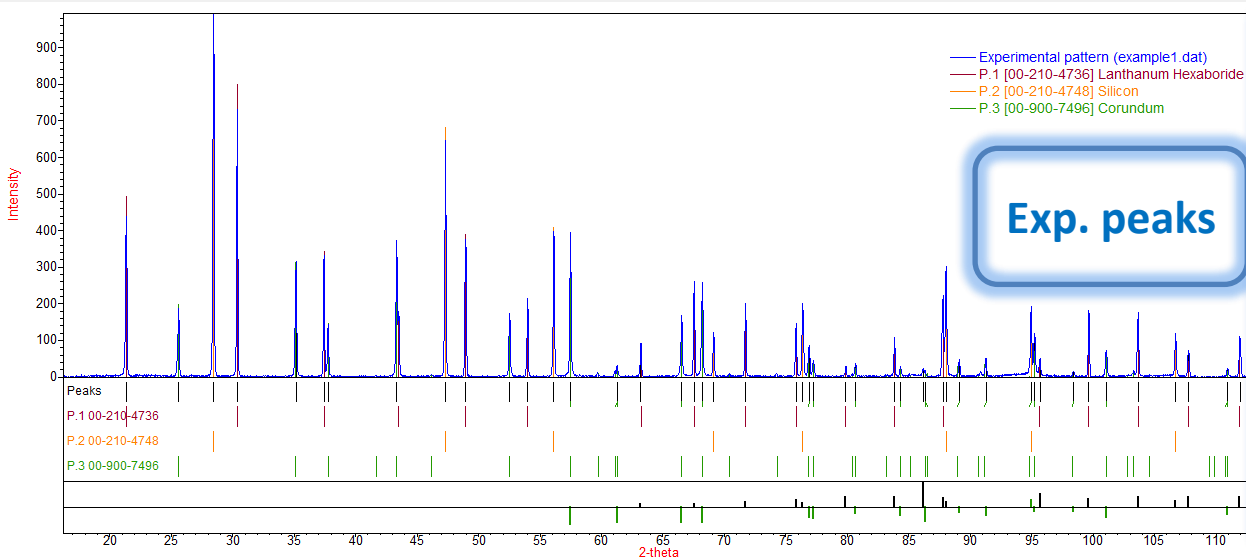
Phase identification using COD with QualX



Found results

QualX - [C:\Program Files\QualX\examples\example1.dat]

File View Pattern Search Help



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	
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

n: 1317 Counts: -388.74 2theta: 54.142 d: 1.693 Estimation of background

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	0.76590	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	
C	00-001-3075	[Bauxite]	Al2 O3	0.68772	0.11242	0.23571E-01	0.52051	6.100	

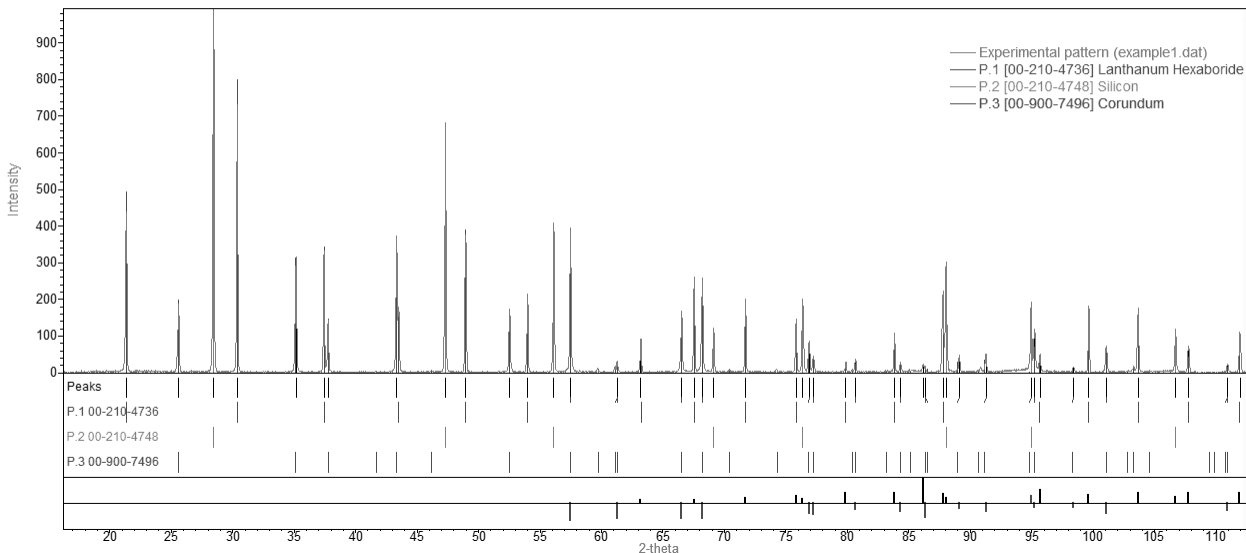
Matched POW_COD C 230 Selected Card 00-900-7496 Al2 O3

Phase identification using COD with QualX



QualX - [C:\Program Files\QualX\examples\example1.dat]

File View Pattern Search Help



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

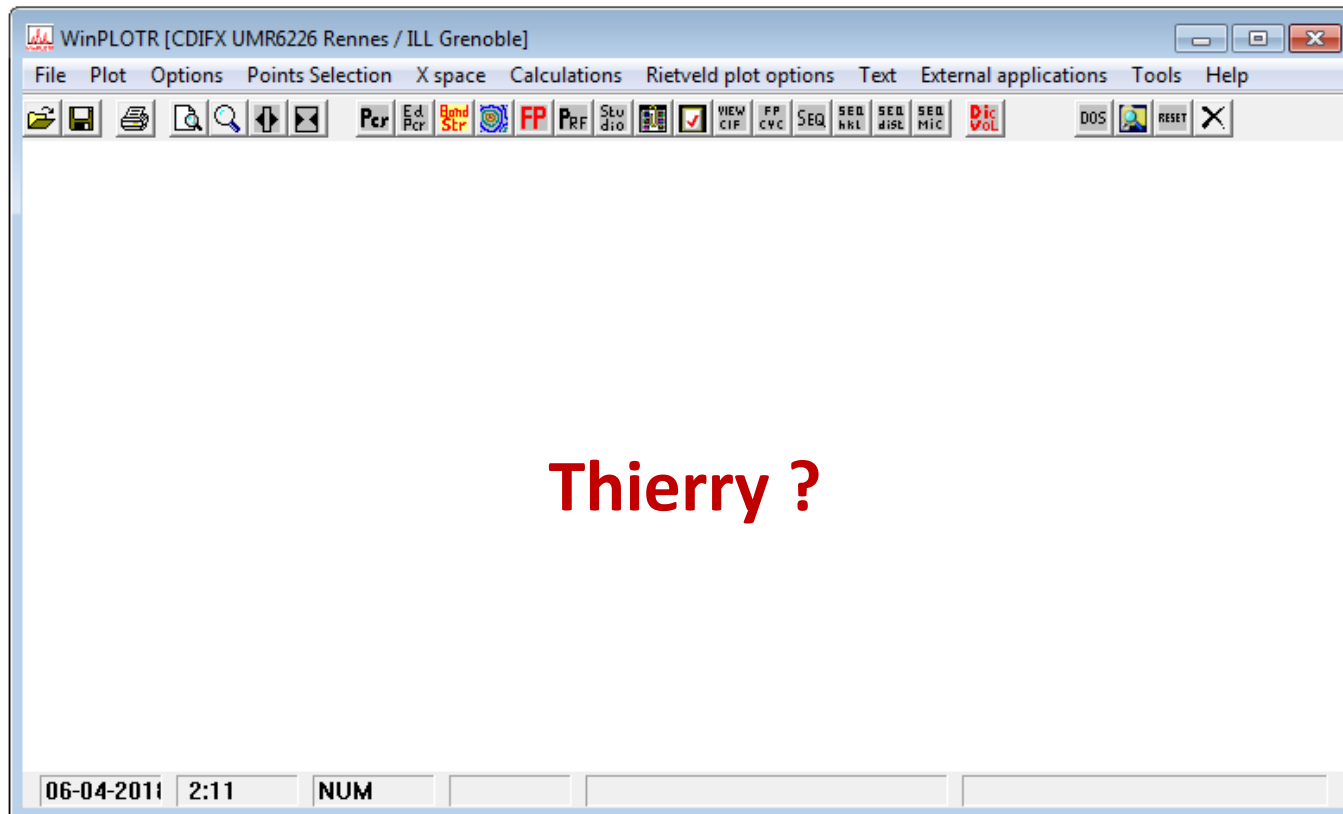
n: 1317 Counts: -388.74 2theta: 54.142 d: 1.693 Estimation of background

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	0.25878	0.29407E-01	0.57545	1.099	✓
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	✓
C	00-001-3075	[Bancalite]	Mn Ni6 O8	0.68772	0.11342	0.23571E-01	0.50951	6.100	✓

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

« Semi quantitative » estimation based on RIR

Phase identification using with Fullprof ?



Thierry ?

Phase identification using

Full Profile Search Match

by L. Lutterotti using 

Phase identification using

Full Profile Search Match

by L. Lutterotti using 

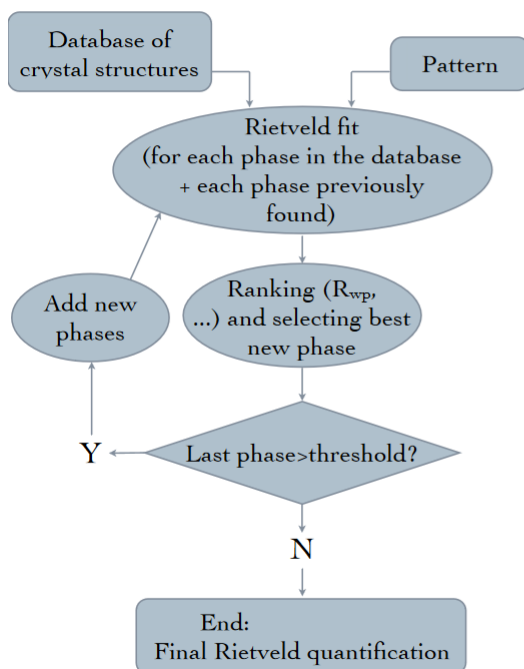
<http://nanoair.dii.unitn.it:8080/sfpm/>

<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

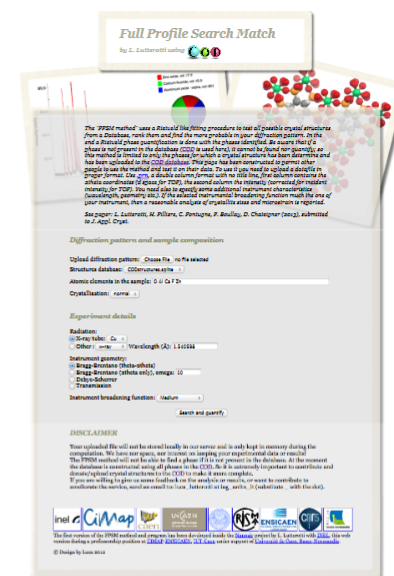


Pro:

- 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.dii.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.

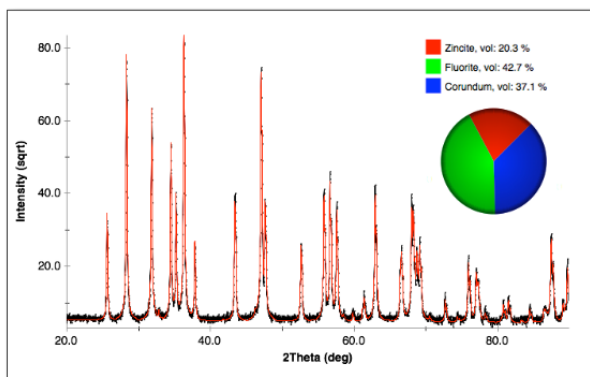
Full Profile Search Match

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 ₂ O ₃	37.1	36.1

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

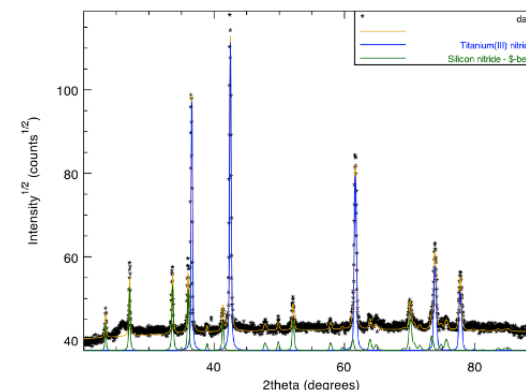
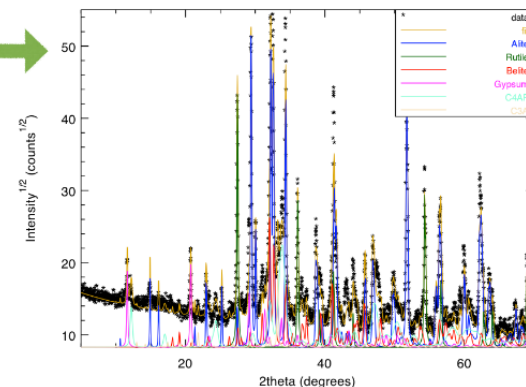
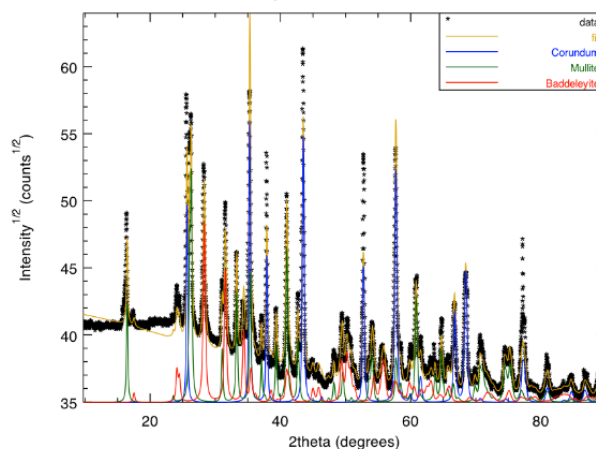
- No composition restriction: **565 secs**
- Only Al, Ca, F, Zn, O, Mg, Na, Si, Cl: **19 secs**

name	vol. (%)	wt. (%)	crystallites (Å)	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 be 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, R_w: 0.045532, GofF: 1.79502



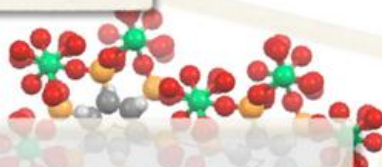
Phase ID	name	vol. (%)	wt. (%)	crystallites (Å)	microstrain
1101045	Titanium(III) nitride	50.0729	62.8891	1682.09	0.00122093
1001246	Silicon nitride - beta	49.9271	37.1109	800.99	0.00129495

Final Rietveld analysis, R_w: 0.0601521, GofF: 2.66024

Full Profile Search Match

by L. Lutterotti using 

Zinc oxide, vol: 17.5
Calcium fluoride, vol: 43.9
Aluminium oxide - alpha, vol: 39.1



The "FPSM method" uses a Rietveld like fitting procedure to test all possible crystal structures from a 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. Be aware that if a phase is not present in the database (*COD* is used here), it cannot be found nor quantify; so this method is limited to only the phases for which a crystal structure has been determined and has been uploaded to the *COD database*. This page has been constructed to permit other people to use the method and test it on their data. To use it you need to upload a datafile in proper format. Use a *.prn* or *.txt*, double column format with no title line, first column contains the 2θ coordinates (d space for TOF), the second column the intensity (corrected for incident intensity for TOF). You need also to specify some additional instrument characteristics (wavelength, geometry etc.). If the selected instrumental broadening function much the one of your instrument, then a reasonable analysis of crystallite sizes and microstrain is reported.

See paper: L. Lutterotti, H. Pilliere, C. Fontugne, P. Boullay, D. Chateigner (2014), submitted to J. Appl. Cryst.

Diffraction pattern and sample composition

Upload diffraction pattern: Aucun fichier sélectionné.

Structures database:

Atomic elements in the sample:

Threshold phase density: Maximum number of phases:

Crystallisation:

Experiment details

Radiation:

☒ X-ray tube:

☐ Other : Wavelength (Å):

Instrument geometry:

☒ Bragg-Brentano (theta-2theta)

☐ Bragg-Brentano (2theta only), omega:

☐ Debye-Scherrer

☐ Transmission

Instrument broadening function:

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)

Full Profile Search Match

by L. Lutterotti using



demonstration

Input file : *.prn 2 columns : (2 θ , 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 ?

- ❑ 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



April 2003, >1200 CIFs



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



Open Access Database



- Add Your Data**
- Deposit your data
- Manage depositions
- Manage/release prepublications

COD Home

- Home
- What's new?

Accessing COD

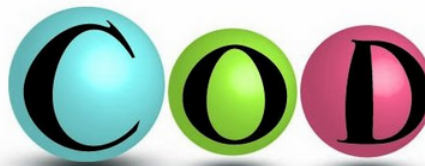
- Browse
- Search
- Search by structural formula

Add Your Data

- Deposit your data
- Manage depositions
- Manage/release prepublications

Documentation

- COD Wiki
- Obtaining CIFs
- Querying COD
- Citing COD
- COD Mirror
- Advice to depositors
- Useful links



Open-access collection of crystal structures of organic, inorganic, metal-organics compounds and minerals, excluding [biopolymers](#).

Including data and software from Crystallography Open Database, developed by Nick Dore at the Department of Chemistry, the University of Cambridge under supervision of [Peter Murray-Rust](#).

Validation and Deposition Interface

Log in

Upload a file

Depositing published structures

A published structure should contain complete bibliographic information: authors' names, journal name, publication year, volume, issue and pages.

If the CIF does not contain the necessary information, you will be asked [to enter](#) it using [the CIF syntax](#). The validator will detect files and data blocks:

Files from commercial databases should not be uploaded without permission.

Data upload

Select CIF or ZIP file with CIFs for check:

Parcourir... Aucun fichier sélectionné.

Validate

But before, you need to create an account...



Crystallograp

COD Home
Home
What's new? 

Accessing COD Data
Browse
Search
Search by structural formula

Add Your Data
Deposit your data
Manage depositions
Manage/release prepublications

Validation and De

[Log in](#)

Depositor login ([sign up](#))

Choose deposition type:
-- choose one --

Username:

Password: ([forgot password](#))

Submit your c

Please fill in your information to create a new account. A star symbol * indicates required fields.

* Your username

New password:

Retype your password:

Password must be at least 8 characters long and contain at least one character from each of the following classes: letters, digits

* Your e-mail:

* Your real name in Latin transliteration (please use only ASCII characters)

Your real name in your national script (please use characters supported by UTF8)

Areas of your scientific interests:

☐ X-ray crystallography ☐ Powder diffraction ☐ Material identification
☐ Software development ☐ Scientific databases ☐ Structural biology
☐ Other (please specify):

Your highest academic degree earned so far:
(none)

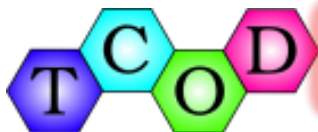
Institution that has awarded the degree:
Name of the institution

Address of the institution:

☐ Je ne suis pas un robot 
reCAPTCHA
Confidentialité - Conditions



extensions ...



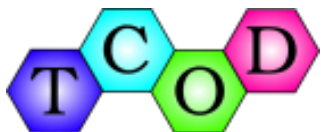
: Theoretical Crystallography Open Database

www.crystallography.net/tcod/

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



extensions ...



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: 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



Material Properties Open Database

[HOME](#)[SEARCH BY ▾](#)[DOCUMENTATION ▾](#)[ABOUT MPOD ▾](#)

Search by Property

PROPERTY
COMPOSITION
REFERENCES

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 eps_{ij}	3,3	1	pure number
dielectric permittivity relative eps_{ij}S	3,3	1	pure number
dielectric permittivity relative eps_{ij}T	3,3	1	pure number
dielectric stiffness relative betri_jS	3,3	10 ⁻⁴	pure number
dielectric stiffness relative betri_jT	3,3	10 ⁻⁴	pure number
elastic TOEC stiffness cij	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 E_{ci}	3	kV.cm ⁻¹	kilovolts per centimetre
electric remnant polarisation P_{ri}	3	10 ⁻⁶ Ohm.cm ⁻²	micro Ohm per square centimetre
electric resistivity rho_{ei}j	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

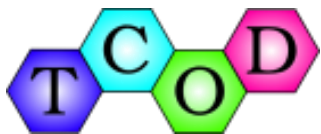
```

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'
data_100 _prop_superconducting_coherence_length_ksii 'ksii'
_cod_dat _prop_superconducting_penetration_depth_lambdai 'lambdai'
_structu _prop_residual_resistivity_ratio 12.4
_phase_1 _prop_residual_resistivity_ratio_high_temperature 300
_phase_1 _prop_residual_resistivity_ratio_low_temperature 4
_chemical loop
_symmetr _prop_data_label
_cell_le _prop_data_tensorial_index
_cell_le _prop_data_value
_cell_le _prop_conditions_temperature
_cell_ar rhoeij 11 110 300
_cell_ar rhoeij 22 110 300
_cell_ar rhoeij 33 ? ?
loop_ rhoeij 11 8.9 4
_publ_ar rhoeij 22 8.9 4
'Ying, C rhoeij 33 ? ?
'Yan, Y. Hc1i 1 0.023 0
'Liu, R. Hc1i 2 0.023 0
'Wang, J Hc1i 3 0.023 0
'Wang, J Hc1i 1 0.0114 1.8
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'Chen, J Hc2i 1 0.114 0
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Isotrop Hirri 1 0.055 1.8
; Hirri 2 0.055 1.8
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_journal ksii 1 54 0
_journal ksii 2 54 0
_journal ksii 3 54 0
_journal lambdai 1 80 0
_journal lambdai 2 80 0
_journal lambdai 3 80 0

```



extensions ...



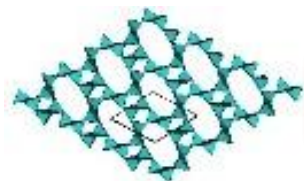
: Theoretical Crystallography Open Database www.crystallography.net/tcod/

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



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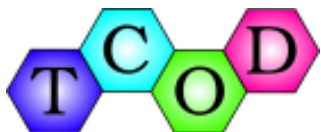


: Predicted Crystallography Open Database <http://www.crystallography.net/pcod/>

- ✓ 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



extensions ...



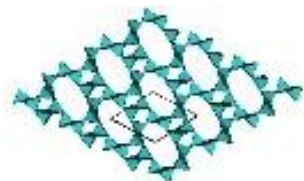
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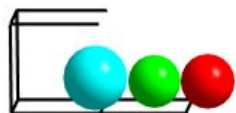
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: Raman Open Database <http://solsa.crystallography.net/rod/>

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





Merci pour votre attention