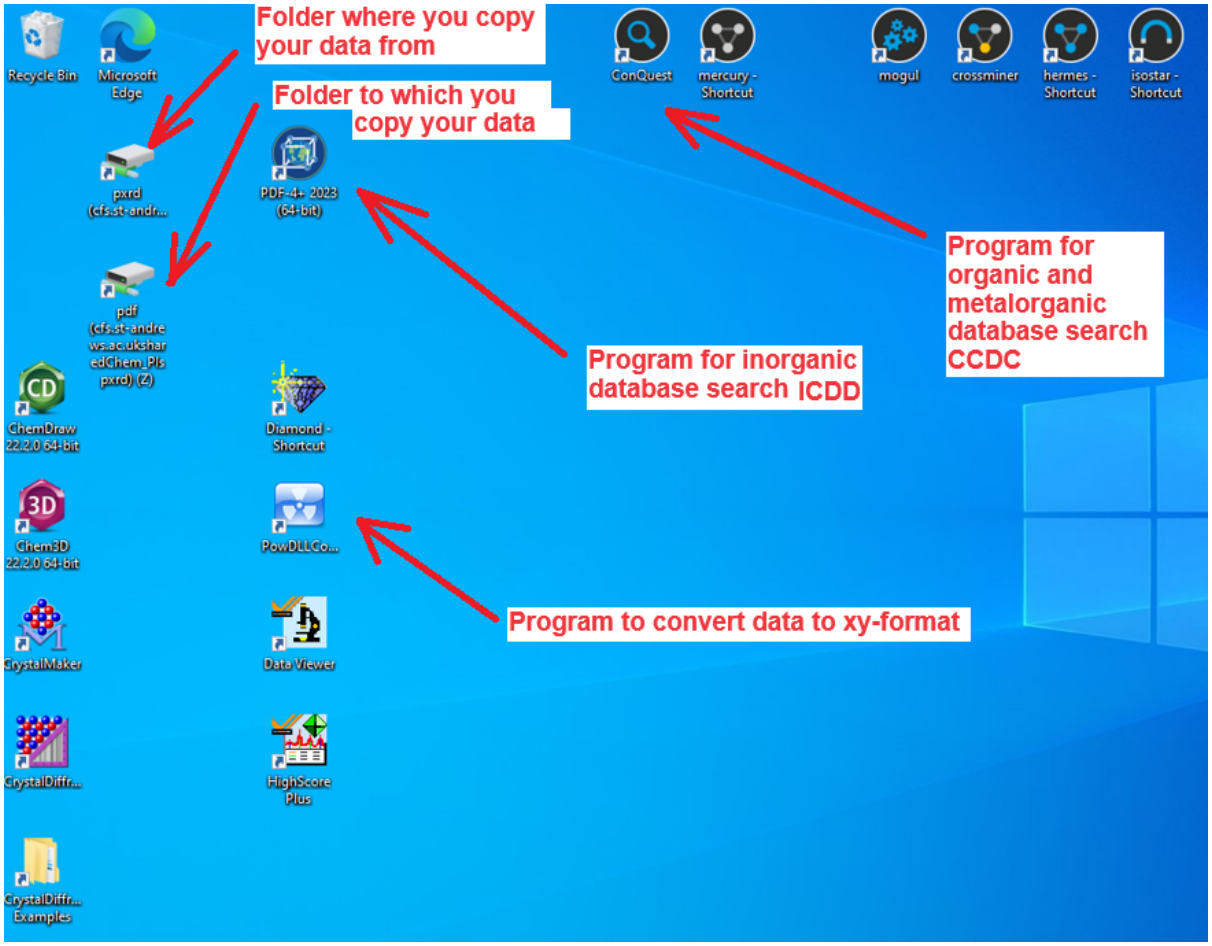
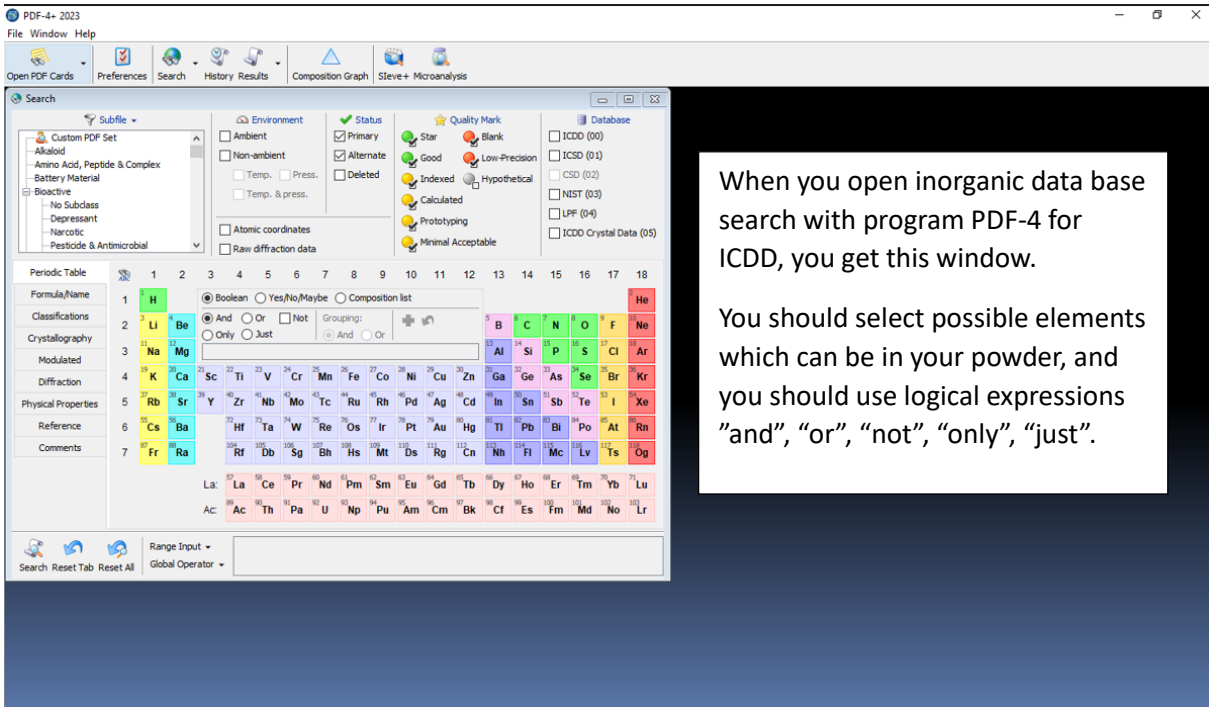
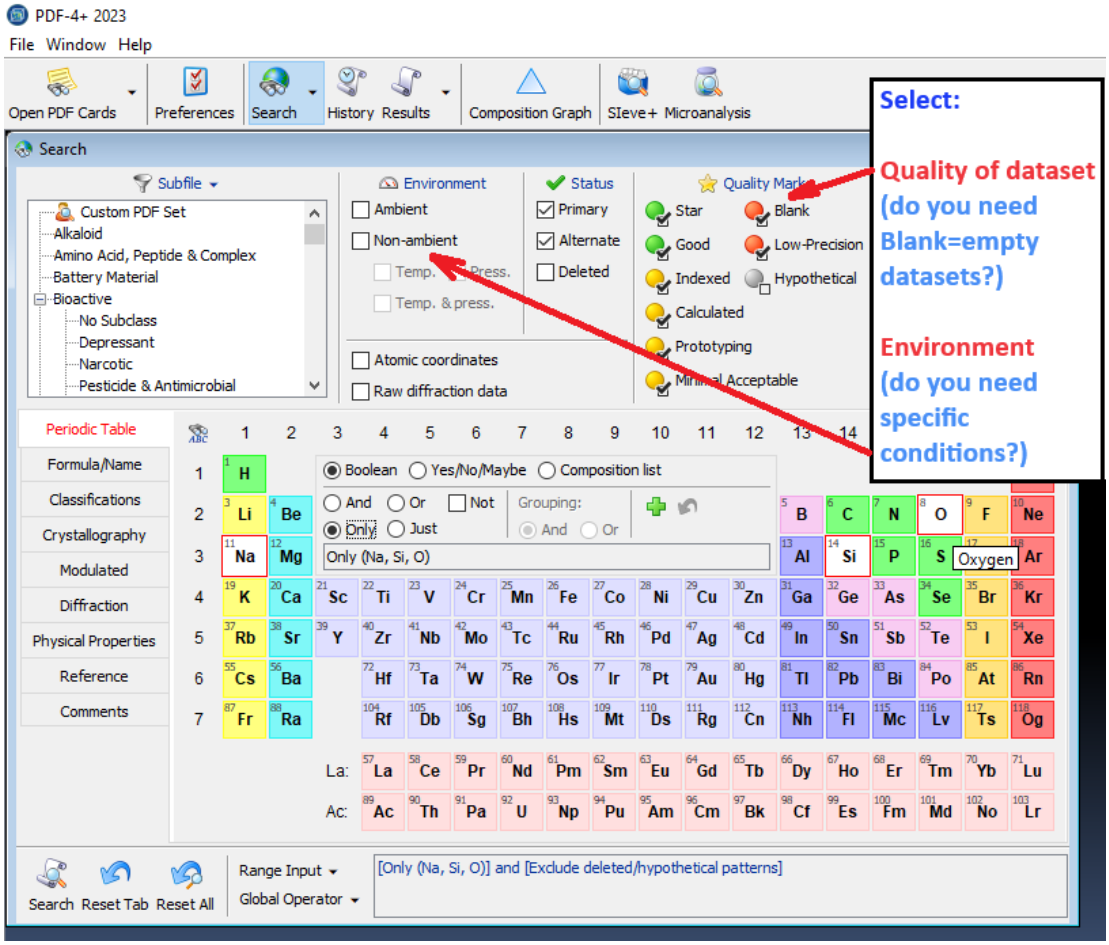
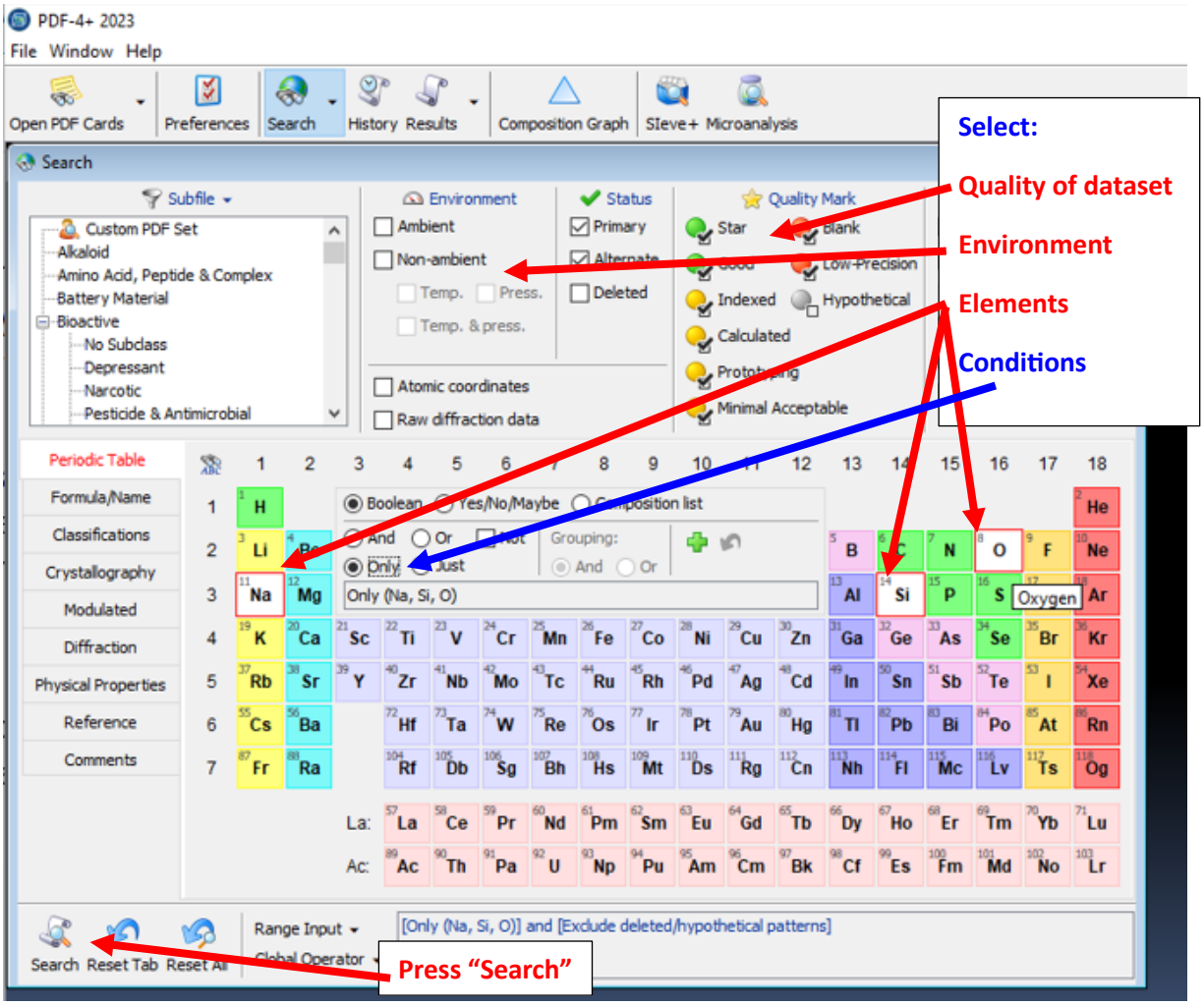


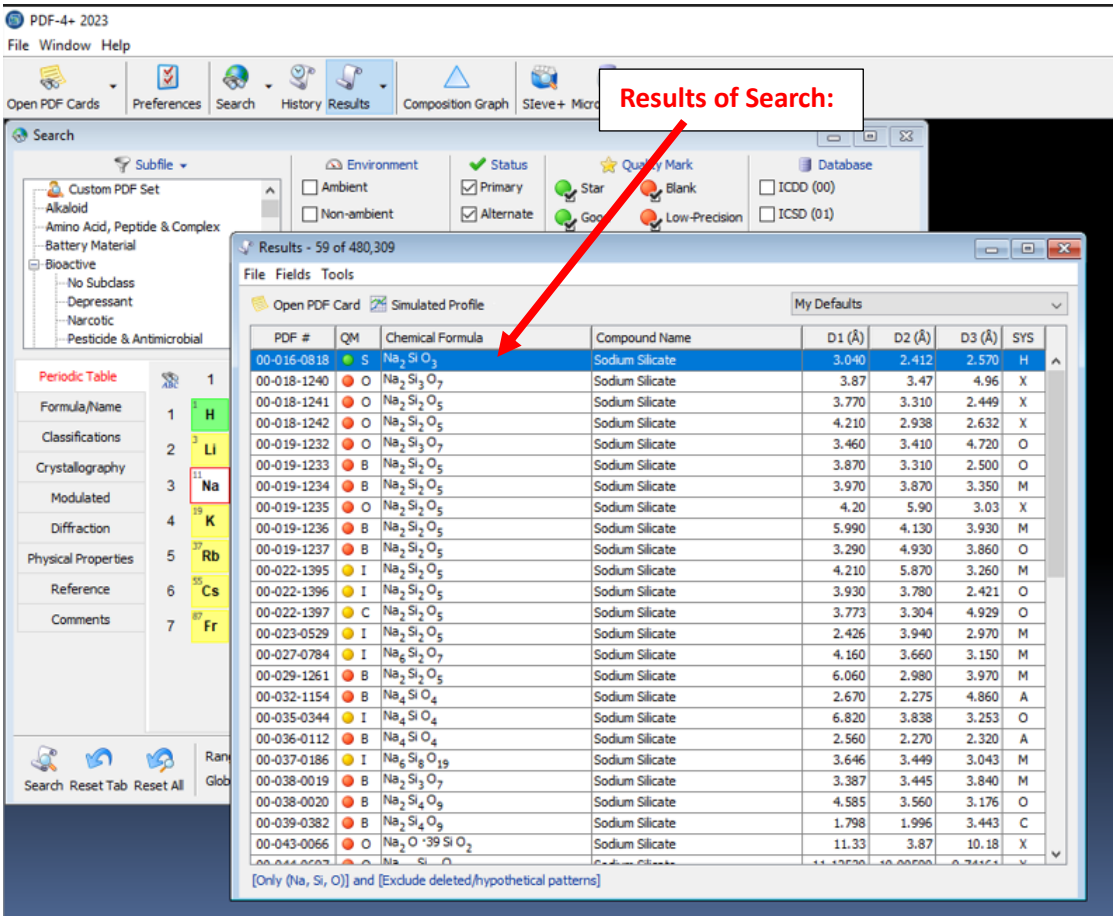


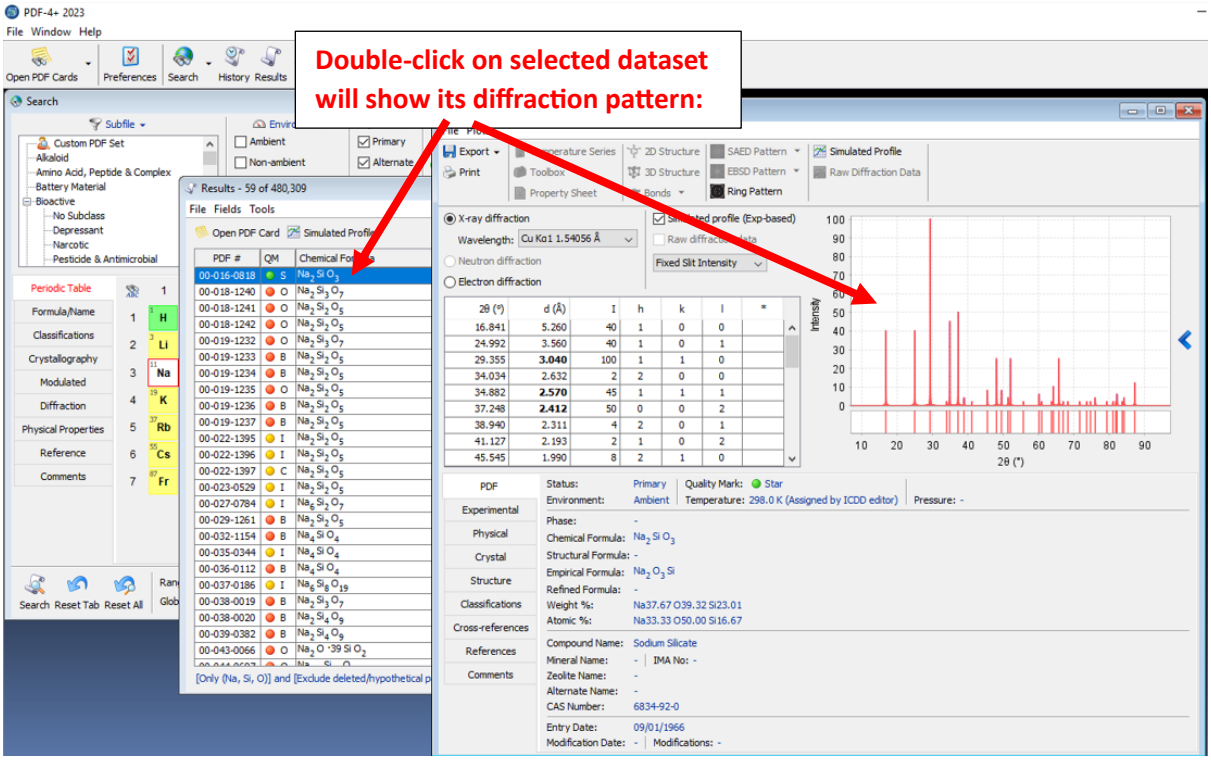
When you open inorganic data base search with program PDF-4 for ICDD, you get this window.

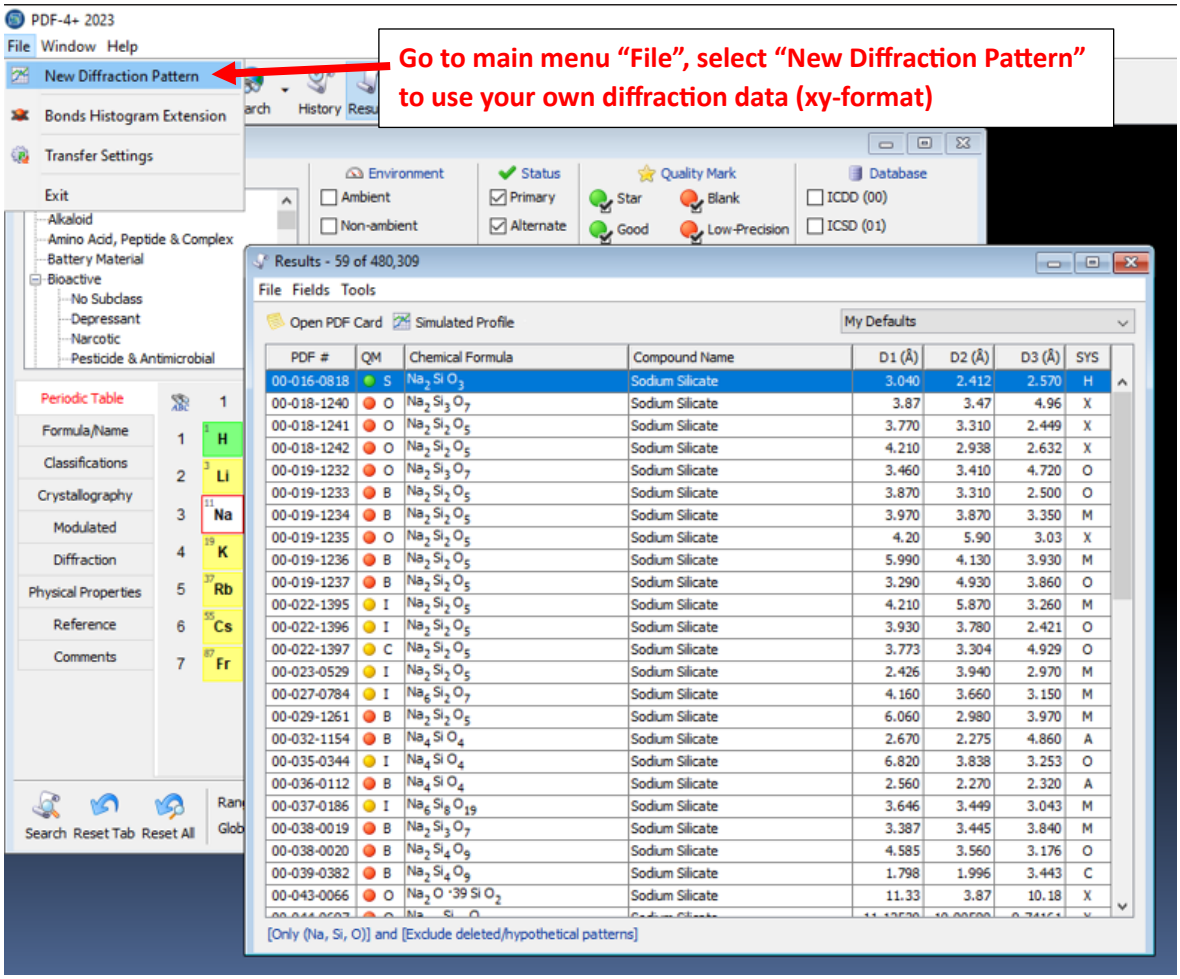
You should select possible elements which can be in your powder, and you should use logical expressions ”and”, “or”, “not”, “only”, “just”.

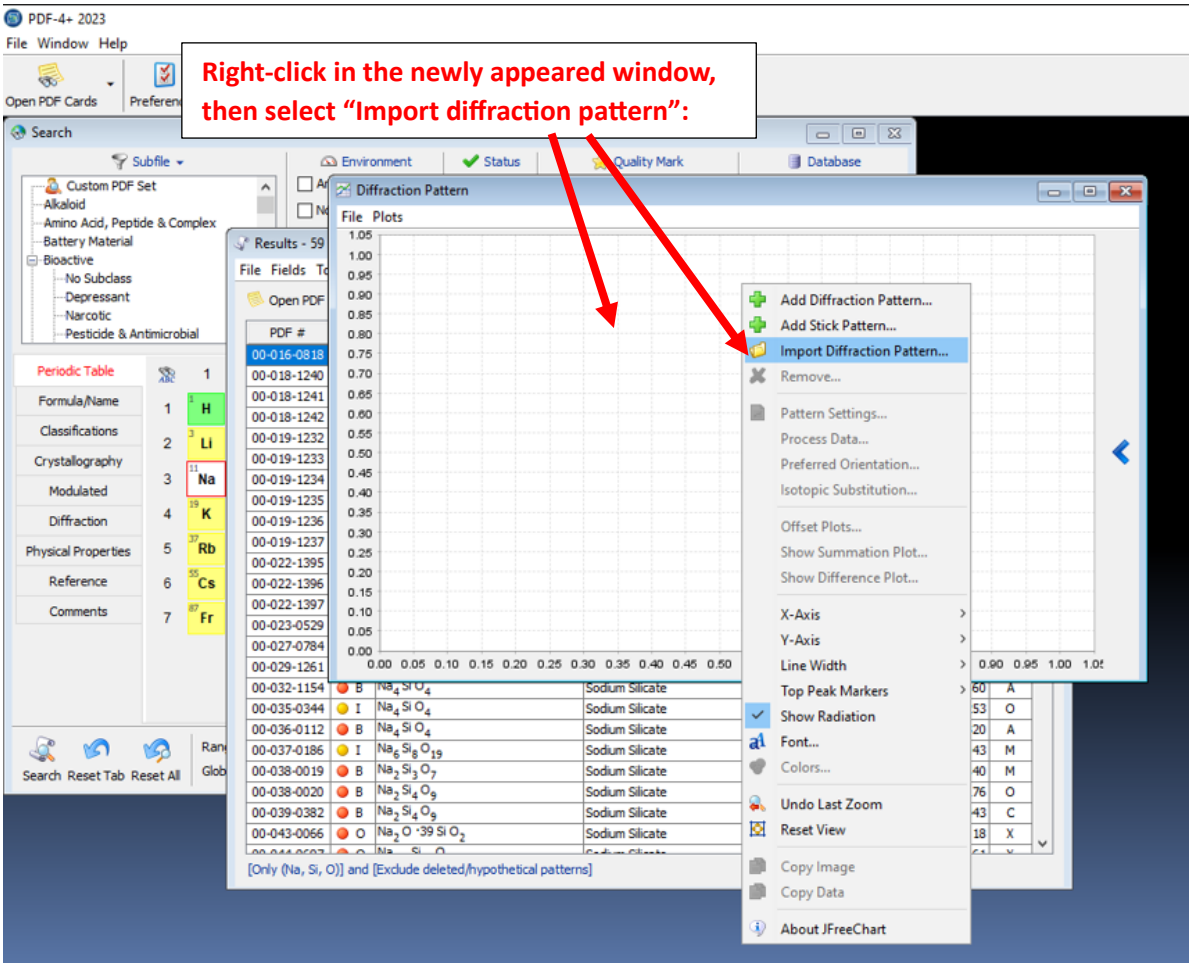

PDF-4+ 2023
File Window Help
Open PDF Cards
Preferences
Search
History
Results
Composition Graph
SIeve+
Microanalysis
Search
Subfile
Custom PDF Set
Alkaloid
Amino Acid, Peptide & Complex
Battery Material
Bioactive
No Subclass
Depressant
Narcotic
Pesticide & Antimicrobial
Environment
Ambient
Non-ambient
Temp.
Press.
Temp. & press.
Atomic coordinates
Raw diffraction data
Status
Primary
Alternate
Deleted
Quality Mark
Star
Blank
Good
Low-Precision
Indexed
Hypothetical
Calculated
Prototyping
Minimal Acceptable
Periodic Table
Formula/Name
Classifications
Crystallography
Modulated
Diffraction
Physical Properties
Reference
Comments
Boolean
Yes/No/Maybe
Composition list
And
Or
Not
Only
Just
Grouping:
And
Or
Only (Na, Si, O)
Oxygen
La:
Ac:
Search
Reset Tab
Reset All
Range Input
Global Operator
[Only (Na, Si, O)] and [Exclude deleted/hypothetical patterns]
Select:
Quality of dataset (do you need Blank=empty datasets?)
Environment (do you need specific conditions?)

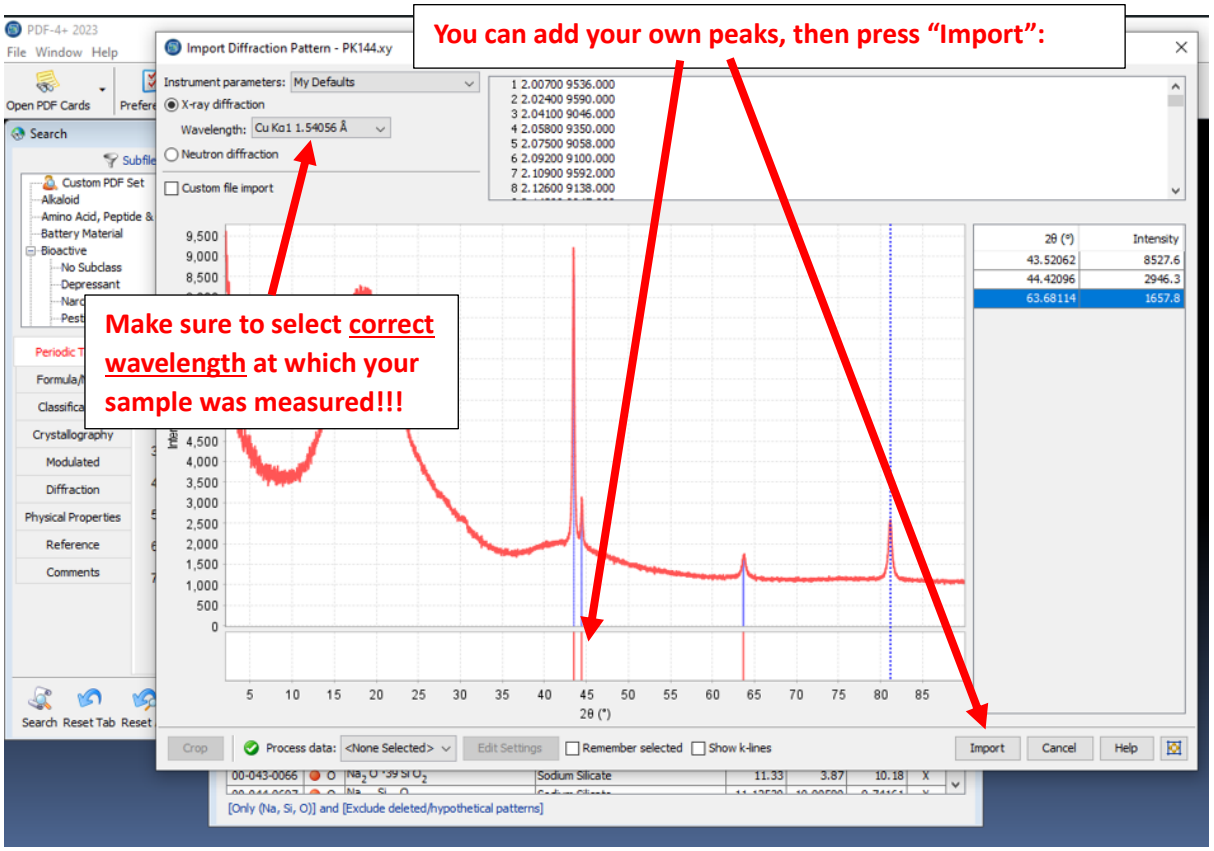

PDF-4+ 2023
File Window Help
Open PDF Cards
Preferences
Search
History
Results
Composition Graph
SIeve+
Microanalysis
Search
Subfile
Custom PDF Set
Alkaloid
Amino Acid, Peptide & Complex
Battery Material
Bioactive
No Subclass
Depressant
Narcotic
Pesticide & Antimicrobial
Environment
Ambient
Non-ambient
Temp.
Press.
Temp. & press.
Atomic coordinates
Raw diffraction data
Status
Primary
Alternate
Deleted
Quality Mark
Star
Blank
Low-Precision
Indexed
Hypothetical
Calculated
Minimal Acceptable
Periodic Table
Formula/Name
Classifications
Crystallography
Modulated
Diffraction
Physical Properties
Reference
Comments
Boolean
And
Or
Only
Just
Grouping:
And
Or
Only (Na, Si, O)
Oxygen
La:
Ac:
Search
Reset Tab
Reset All
Range Input
Global Operator
[Only (Na, Si, O)] and [Exclude deleted/hypothetical patterns]
Select:
Quality of dataset
Environment
Elements
Conditions
Press "Search"

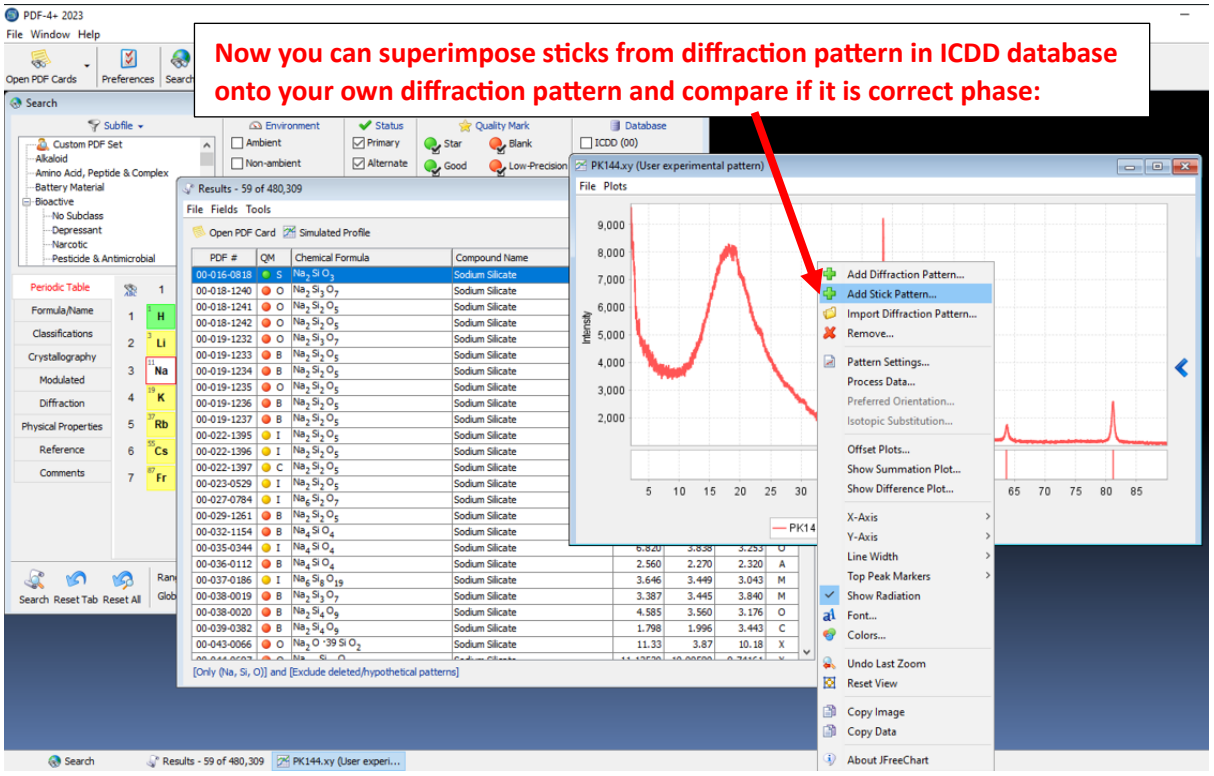

PDF-4+ 2023
File Window Help
Open PDF Cards
Preferences
Search
History
Results
Composition Graph
Results of Search:
Search
Subfile
Custom PDF Set
Alkaloid
Amino Acid, Peptide & Complex
Battery Material
Bioactive
No Subclass
Depressant
Narcotic
Pesticide & Antimicrobial
Environment
Ambient
Non-ambient
Status
Primary
Alternate
Quality Mark
Star
Blank
Low-Precision
Database
ICDD (00)
ICSD (01)
Periodic Table
Formula/Name
Classifications
Crystallography
Modulated
Diffraction
Physical Properties
Reference
Comments
Search
Reset Tab
Reset All
Results - 59 of 480,309
File Fields Tools
Open PDF Card
Simulated Profile
My Defaults
PDF # | QM | Chemical Formula | Compound Name | D1 (Å) | D2 (Å) | D3 (Å) | SYS
00-016-0818 | S | $Na_2Si_2O_3$ | Sodium Silicate | 3.040 | 2.412 | 2.570 | H
00-018-1240 | O | $Na_2Si_3O_7$ | Sodium Silicate | 3.87 | 3.47 | 4.96 | X
00-018-1241 | O | $Na_2Si_2O_5$ | Sodium Silicate | 3.770 | 3.310 | 2.449 | X
00-018-1242 | O | $Na_2Si_2O_5$ | Sodium Silicate | 4.210 | 2.938 | 2.632 | X
00-019-1232 | O | $Na_2Si_3O_7$ | Sodium Silicate | 3.460 | 3.410 | 4.720 | O
00-019-1233 | B | $Na_2Si_2O_5$ | Sodium Silicate | 3.870 | 3.310 | 2.500 | O
00-019-1234 | B | $Na_2Si_2O_5$ | Sodium Silicate | 3.970 | 3.870 | 3.350 | M
00-019-1235 | O | $Na_2Si_2O_5$ | Sodium Silicate | 4.20 | 5.90 | 3.03 | X
00-019-1236 | B | $Na_2Si_2O_5$ | Sodium Silicate | 5.990 | 4.130 | 3.930 | M
00-019-1237 | B | $Na_2Si_2O_5$ | Sodium Silicate | 3.290 | 4.930 | 3.860 | O
00-022-1395 | I | $Na_2Si_2O_5$ | Sodium Silicate | 4.210 | 5.870 | 3.260 | M
00-022-1396 | I | $Na_2Si_2O_5$ | Sodium Silicate | 3.930 | 3.780 | 2.421 | O
00-022-1397 | C | $Na_2Si_2O_5$ | Sodium Silicate | 3.773 | 3.304 | 4.929 | O
00-023-0529 | I | $Na_2Si_2O_5$ | Sodium Silicate | 2.426 | 3.940 | 2.970 | M
00-027-0784 | I | $Na_6Si_2O_7$ | Sodium Silicate | 4.160 | 3.660 | 3.150 | M
00-029-1261 | B | $Na_2Si_2O_5$ | Sodium Silicate | 6.060 | 2.980 | 3.970 | M
00-032-1154 | B | Na_4SiO_4 | Sodium Silicate | 2.670 | 2.275 | 4.860 | A
00-035-0344 | I | Na_4SiO_4 | Sodium Silicate | 6.820 | 3.838 | 3.253 | O
00-036-0112 | B | Na_4SiO_4 | Sodium Silicate | 2.560 | 2.270 | 2.320 | A
00-037-0186 | I | $Na_6Si_8O_{19}$ | Sodium Silicate | 3.646 | 3.449 | 3.043 | M
00-038-0019 | B | $Na_2Si_3O_7$ | Sodium Silicate | 3.387 | 3.445 | 3.840 | M
00-038-0020 | B | $Na_2Si_4O_9$ | Sodium Silicate | 4.585 | 3.560 | 3.176 | O
00-039-0382 | B | $Na_2Si_4O_9$ | Sodium Silicate | 1.798 | 1.996 | 3.443 | C
00-043-0066 | O | $Na_2O \cdot 39\,SiO_2$ | Sodium Silicate | 11.33 | 3.87 | 10.18 | X
[Only (Na, Si, O)] and [Exclude deleted/hypothetical patterns]

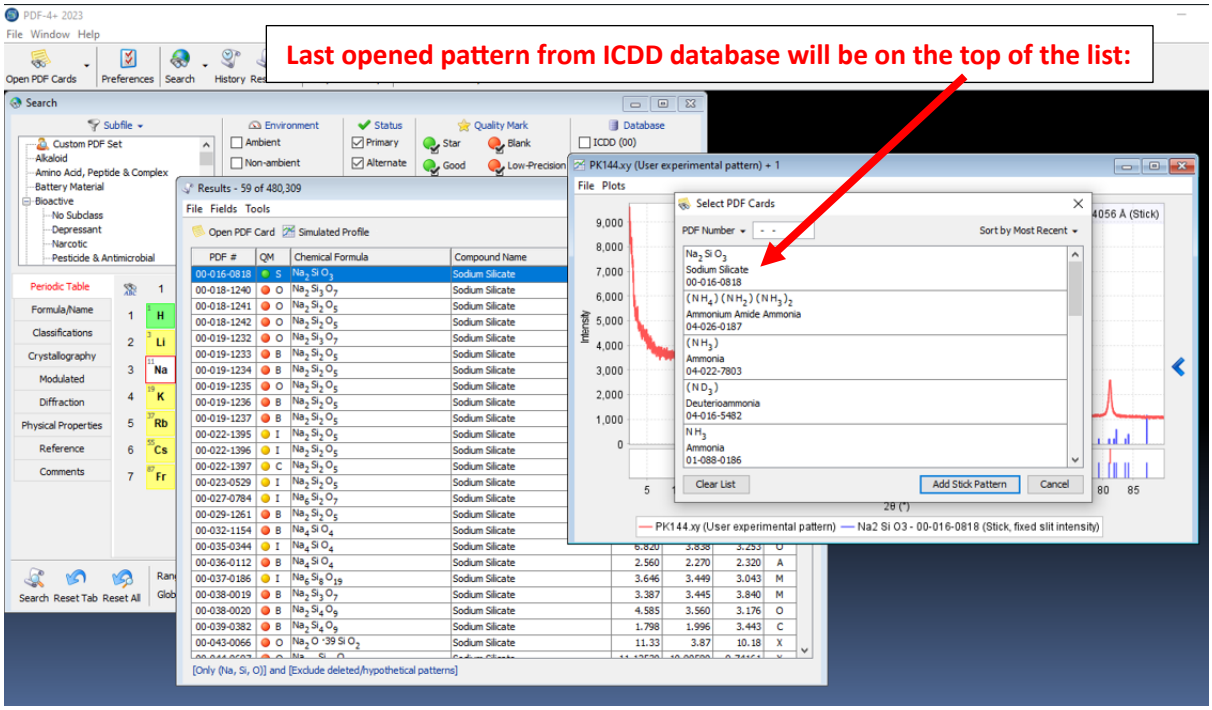

PDF-4+ 2023
File Window Help
Double-click on selected dataset
will show its diffraction pattern:
Search
Results - 59 of 480,309
File Fields Tools
Export
Print
Simulated Profile
Raw Diffraction Data
X-ray diffraction
Neutron diffraction
Electron diffraction
Wavelength: Cu Ka1 1.54056 Å
Fixed Slit Intensity
2θ (°) | d (Å) | I | h | k | l
16.841 | 5.260 | 40 | 1 | 0 | 0
24.992 | 3.560 | 40 | 1 | 0 | 1
29.355 | 3.040 | 100 | 1 | 1 | 0
34.034 | 2.632 | 2 | 2 | 0 | 0
34.882 | 2.570 | 45 | 1 | 1 | 1
37.248 | 2.412 | 50 | 0 | 0 | 2
38.940 | 2.311 | 4 | 2 | 0 | 1
41.127 | 2.193 | 2 | 1 | 0 | 2
45.545 | 1.990 | 8 | 2 | 1 | 0
Intensity
2θ (°)
PDF
Experimental
Physical
Crystal
Structure
Classifications
Cross-references
References
Comments
Status: Primary
Quality Mark: Star
Environment: Ambient
Temperature: 298.0 K (Assigned by ICDD editor)
Pressure: -
Phase: -
Chemical Formula: $Na_2Si_2O_3$
Structural Formula: -
Empirical Formula: Na_2O_3Si
Refined Formula: -
Weight %: Na37.67 O39.32 Si23.01
Atomic %: Na33.33 O50.00 Si16.67
Compound Name: Sodium Silicate
Mineral Name: - | IMA No: -
Zeolite Name: -
Alternate Name: -
CAS Number: 6834-92-0
Entry Date: 09/01/1966
Modification Date: - | Modifications: -

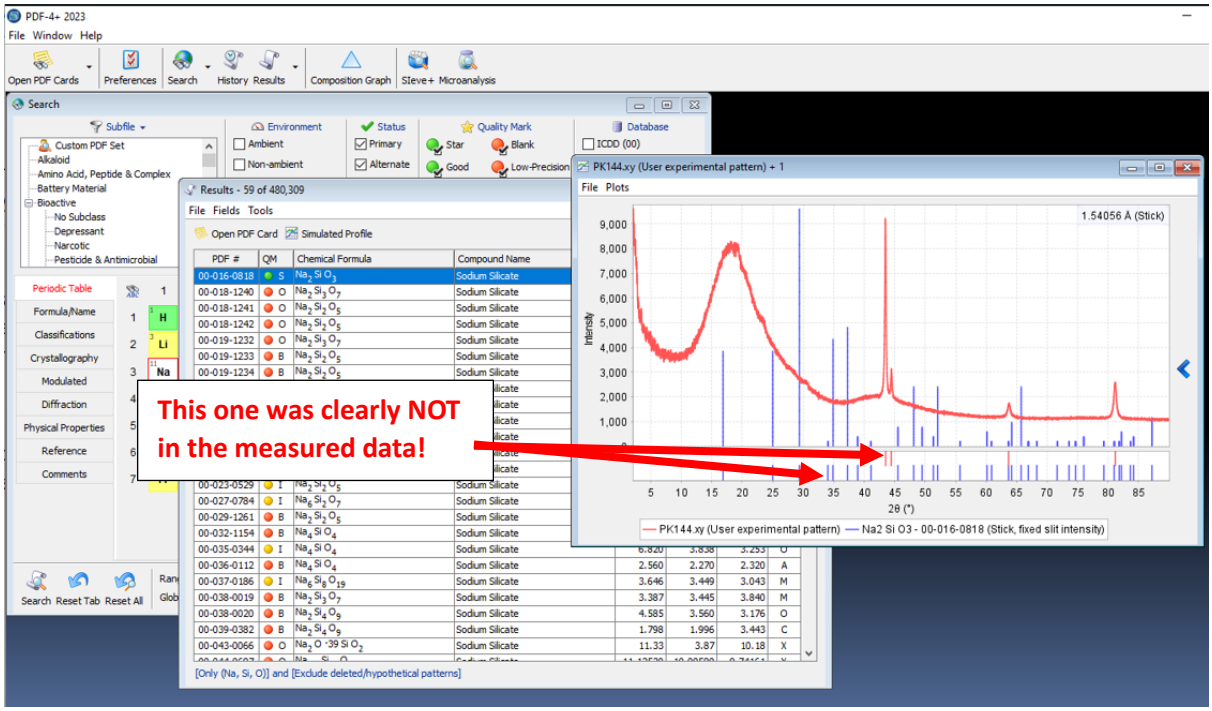

PDF-4+ 2023
File Window Help
New Diffraction Pattern
Bonds Histogram Extension
Transfer Settings
Exit
Go to main menu “File”, select “New Diffraction Pattern” to use your own diffraction data (xy-format)
Environment
Ambient
Non-ambient
Status
Primary
Alternate
Quality Mark
Star
Good
Blank
Low-Precision
Database
ICDD (00)
ICSD (01)
Alkaloid
Amino Acid, Peptide & Complex
Battery Material
Bioactive
No Subclass
Depressant
Narcotic
Pesticide & Antimicrobial
Periodic Table
Formula/Name
Classifications
Crystallography
Modulated
Diffraction
Physical Properties
Reference
Comments
Search
Reset Tab
Reset All
Results - 59 of 480,309
File Fields Tools
Open PDF Card
Simulated Profile
My Defaults
PDF # | QM | Chemical Formula | Compound Name | D1 (Å) | D2 (Å) | D3 (Å) | SYS
00-016-0818 | S | Na2Si O3 | Sodium Silicate | 3.040 | 2.412 | 2.570 | H
00-018-1240 | O | Na2Si3O7 | Sodium Silicate | 3.87 | 3.47 | 4.96 | X
00-018-1241 | O | Na2Si2O5 | Sodium Silicate | 3.770 | 3.310 | 2.449 | X
00-018-1242 | O | Na2Si2O5 | Sodium Silicate | 4.210 | 2.938 | 2.632 | X
00-019-1232 | O | Na2Si3O7 | Sodium Silicate | 3.460 | 3.410 | 4.720 | O
00-019-1233 | B | Na2Si2O5 | Sodium Silicate | 3.870 | 3.310 | 2.500 | O
00-019-1234 | B | Na2Si2O5 | Sodium Silicate | 3.970 | 3.870 | 3.350 | M
00-019-1235 | O | Na2Si2O5 | Sodium Silicate | 4.20 | 5.90 | 3.03 | X
00-019-1236 | B | Na2Si2O5 | Sodium Silicate | 5.990 | 4.130 | 3.930 | M
00-019-1237 | B | Na2Si2O5 | Sodium Silicate | 3.290 | 4.930 | 3.860 | O
00-022-1395 | I | Na2Si2O5 | Sodium Silicate | 4.210 | 5.870 | 3.260 | M
00-022-1396 | I | Na2Si2O5 | Sodium Silicate | 3.930 | 3.780 | 2.421 | O
00-022-1397 | C | Na2Si2O5 | Sodium Silicate | 3.773 | 3.304 | 4.929 | O
00-023-0529 | I | Na2Si2O5 | Sodium Silicate | 2.426 | 3.940 | 2.970 | M
00-027-0784 | I | Na6Si2O7 | Sodium Silicate | 4.160 | 3.660 | 3.150 | M
00-029-1261 | B | Na2Si2O5 | Sodium Silicate | 6.060 | 2.980 | 3.970 | M
00-032-1154 | B | Na4SiO4 | Sodium Silicate | 2.670 | 2.275 | 4.860 | A
00-035-0344 | I | Na4SiO4 | Sodium Silicate | 6.820 | 3.838 | 3.253 | O
00-036-0112 | B | Na4SiO4 | Sodium Silicate | 2.560 | 2.270 | 2.320 | A
00-037-0186 | I | Na6Si8O19 | Sodium Silicate | 3.646 | 3.449 | 3.043 | M
00-038-0019 | B | Na2Si3O7 | Sodium Silicate | 3.387 | 3.445 | 3.840 | M
00-038-0020 | B | Na2Si4O9 | Sodium Silicate | 4.585 | 3.560 | 3.176 | O
00-039-0382 | B | Na2Si4O9 | Sodium Silicate | 1.798 | 1.996 | 3.443 | C
00-043-0066 | O | Na2O ·39 SiO2 | Sodium Silicate | 11.33 | 3.87 | 10.18 | X
[Only (Na, Si, O)] and [Exclude deleted/hypothetical patterns]

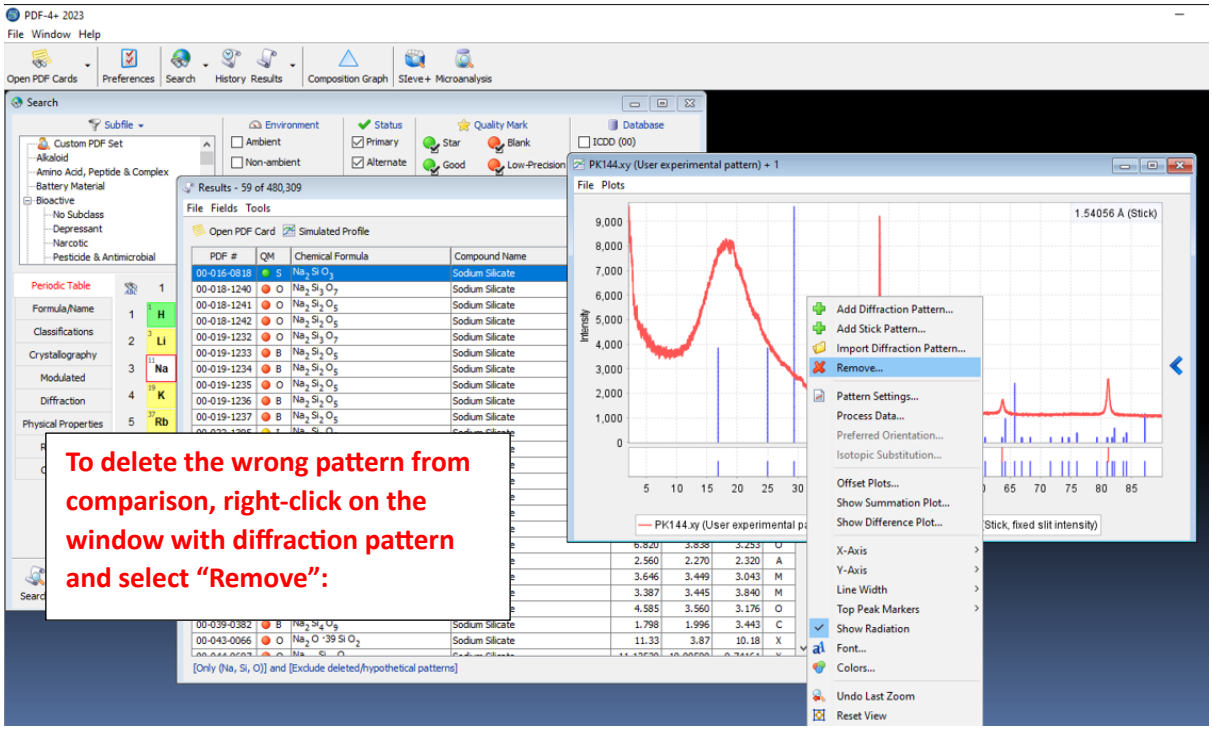

PDF-4+ 2023
File Window Help
Open PDF Cards
Right-click in the newly appeared window, then select “Import diffraction pattern”:
Search
Diffraction Pattern
File Plots
Add Diffraction Pattern...
Add Stick Pattern...
Import Diffraction Pattern...
Remove...
Pattern Settings...
Process Data...
Preferred Orientation...
Isotopic Substitution...
Offset Plots...
Show Summation Plot...
Show Difference Plot...
X-Axis
Y-Axis
Line Width
Top Peak Markers
Show Radiation
Font...
Colors...
Undo Last Zoom
Reset View
Copy Image
Copy Data
About JFreeChart
Custom PDF Set
Alkaloid
Amino Acid, Peptide & Complex
Battery Material
Bioactive
No Subclass
Depressant
Narcotic
Pesticide & Antimicrobial
Periodic Table
Formula/Name
Classifications
Crystallography
Modulated
Diffraction
Physical Properties
Reference
Comments
Search
Reset Tab
Reset All
[Only (Na, Si, O)] and [Exclude deleted/hypothetical patterns]

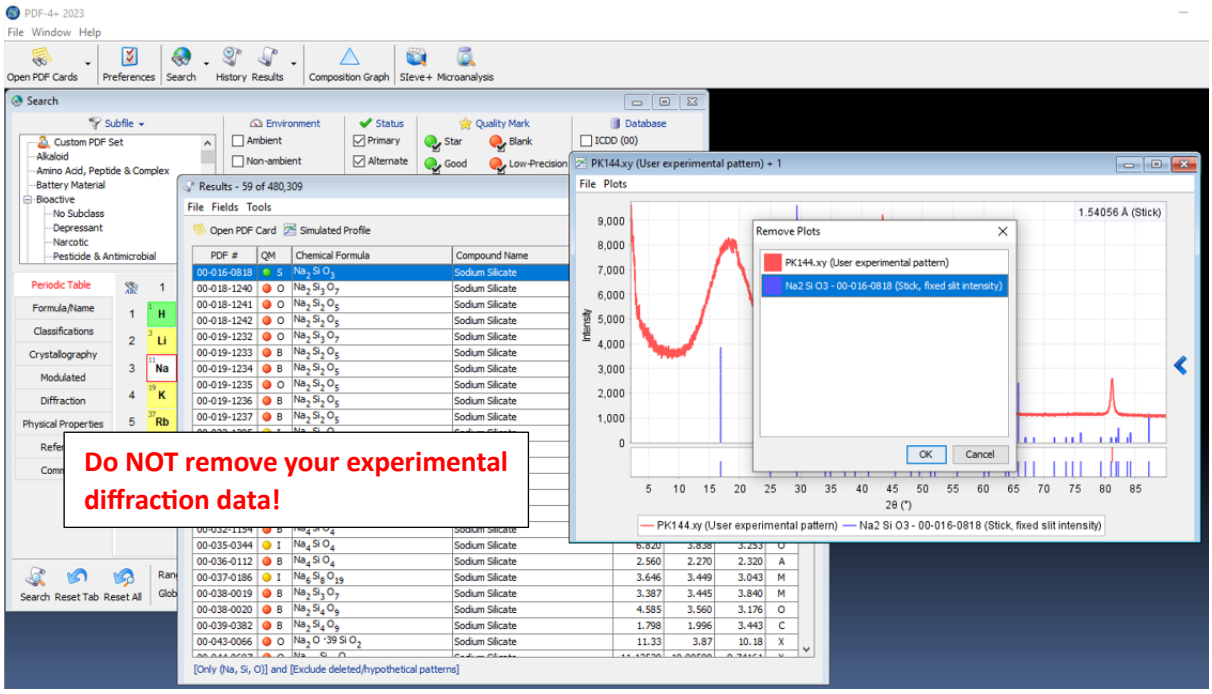

You can add your own peaks, then press “Import”:
Make sure to select correct wavelength at which your sample was measured!!!
Import Diffraction Pattern - PK144.xy
Instrument parameters: My Defaults
X-ray diffraction
Wavelength: Cu Kα1 1.54056 Å
Neutron diffraction
Custom file import
1 2.00700 9536.000
2 2.02400 9590.000
3 2.04100 9046.000
4 2.05800 9350.000
5 2.07500 9058.000
6 2.09200 9100.000
7 2.10900 9592.000
8 2.12600 9138.000
2θ (°)
Intensity
43.52062 8527.6
44.42096 2946.3
63.68114 1657.8
Crop
Process data: <None Selected>
Edit Settings
Remember selected
Show k-lines
Import
Cancel
Help
[Only (Na, Si, O)] and [Exclude deleted/hypothetical patterns]

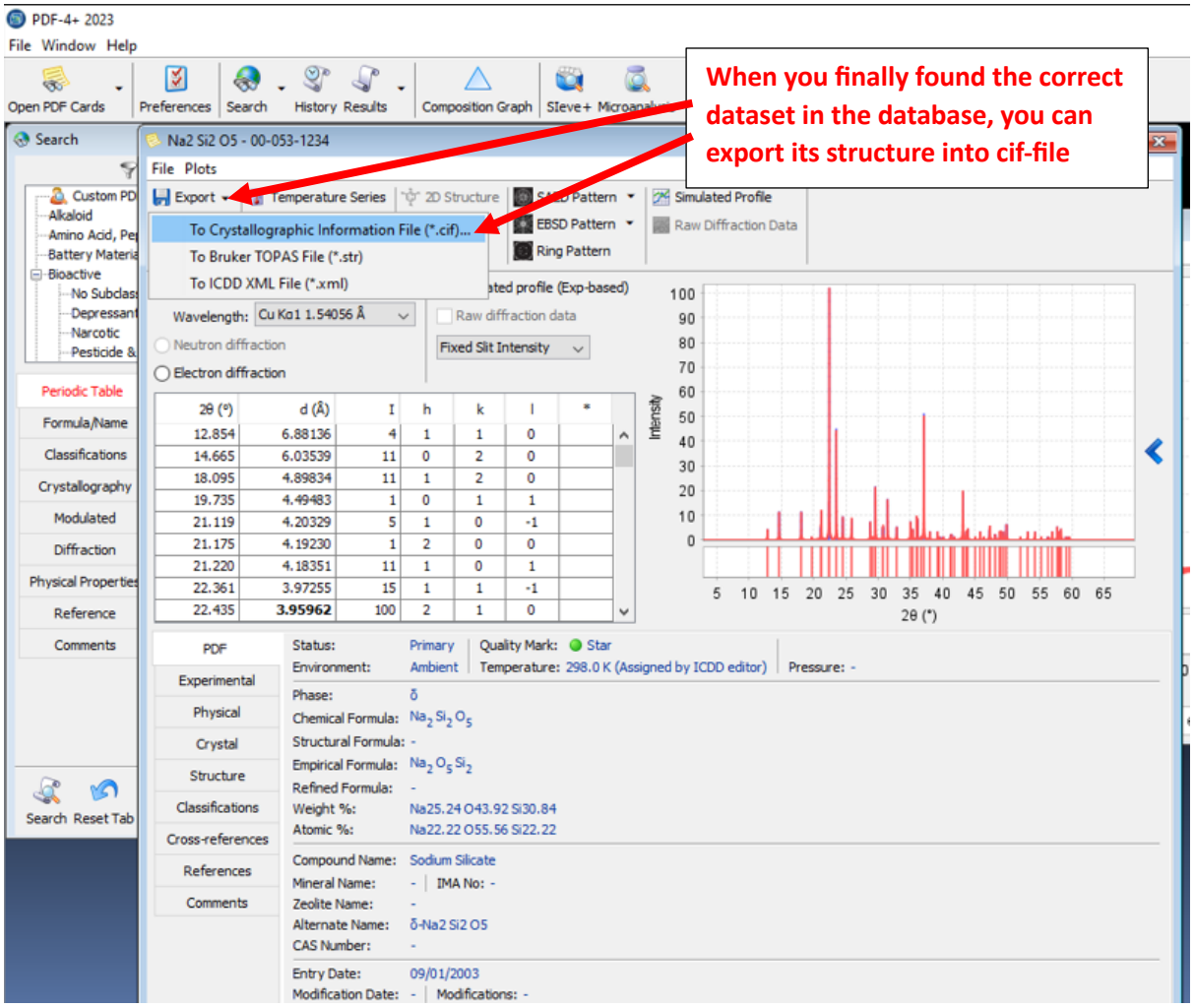

Now you can superimpose sticks from diffraction pattern in ICDD database onto your own diffraction pattern and compare if it is correct phase:
Results - 59 of 480,309
PK144.xy (User experimental pattern)
Add Diffraction Pattern...
Add Stick Pattern...
Import Diffraction Pattern...
Remove...
Pattern Settings...
Process Data...
Preferred Orientation...
Isotopic Substitution...
Offset Plots...
Show Summation Plot...
Show Difference Plot...
X-Axis
Y-Axis
Line Width
Top Peak Markers
Show Radiation
Font...
Colors...
Undo Last Zoom
Reset View
Copy Image
Copy Data
About JFreeChart
[Only (Na, Si, O)] and [Exclude deleted/hypothetical patterns]

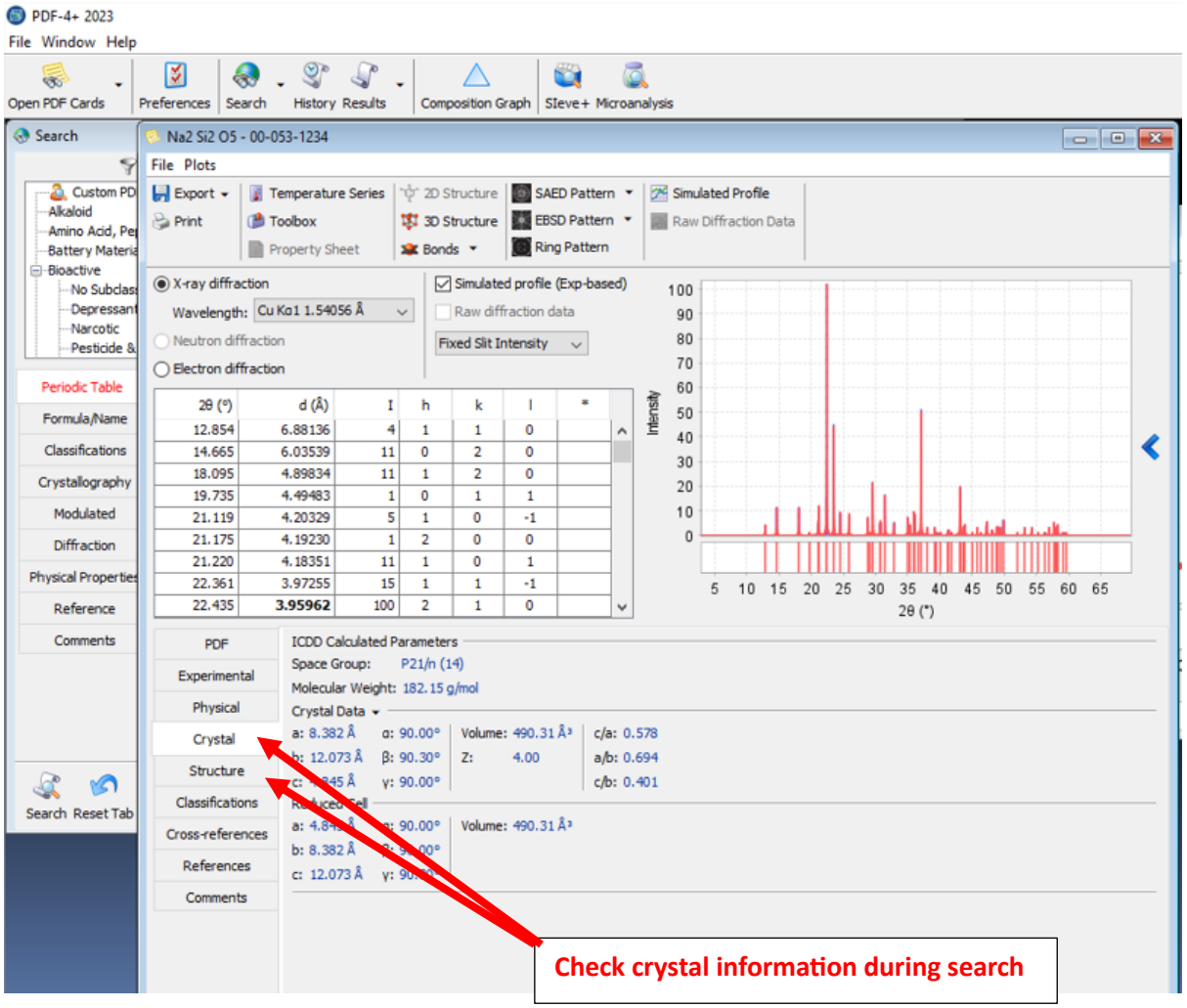

Last opened pattern from ICDD database will be on the top of the list:
PDF-4+ 2023
File Window Help
Open PDF Cards
Preferences
Search
History
Search
Subfile
Environment
Status
Quality Mark
Database
Custom PDF Set
Alkaloid
Amino Acid, Peptide & Complex
Battery Material
Bioactive
No Subclass
Depressant
Narcotic
Pesticide & Antimicrobial
Ambient
Non-ambient
Primary
Alternate
Star
Blank
Good
Low-Precision
ICDD (00)
Periodic Table
Formula/Name
Classifications
Crystallography
Modulated
Diffraction
Physical Properties
Reference
Comments
Search
Reset Tab
Reset All
Results - 59 of 480,309
File Fields Tools
Open PDF Card
Simulated Profile
PDF #
QM
Chemical Formula
Compound Name
00-016-0818
00-018-1240
00-018-1241
00-018-1242
00-019-1232
00-019-1233
00-019-1234
00-019-1235
00-019-1236
00-019-1237
00-022-1395
00-022-1396
00-022-1397
00-023-0529
00-027-0784
00-029-1261
00-032-1154
00-035-0344
00-036-0112
00-037-0186
00-038-0019
00-038-0020
00-039-0382
00-043-0066
Sodium Silicate
[Only (Na, Si, O)] and [Exclude deleted/hypothetical patterns]
PK144.xy (User experimental pattern) + 1
File Plots
Select PDF Cards
PDF Number
Sort by Most Recent
Sodium Silicate
00-016-0818
Ammonium Amide Ammonia
04-026-0187
Ammonia
04-022-7803
Deuterioammonia
04-016-5482
Ammonia
01-088-0186
Clear List
Add Stick Pattern
Cancel
4056 Å (Stick)
Intensity
2θ (°)
PK144.xy (User experimental pattern)
Na2 Si O3 - 00-016-0818 (Stick, fixed slit intensity)


PDF-4+ 2023
File Window Help
Open PDF Cards
Preferences
Search
History
Results
Composition Graph
SIeve+
Microanalysis
This one was clearly NOT
in the measured data!
PK144.xy (User experimental pattern) + 1
File Plots
1.54056 Å (Stick)
Intensity
2θ (°)
PK144.xy (User experimental pattern)
Na2 Si O3 - 00-016-0818 (Stick, fixed slit intensity)


To delete the wrong pattern from comparison, right-click on the window with diffraction pattern and select “Remove”:


Do NOT remove your experimental diffraction data!


When you finally found the correct dataset in the database, you can export its structure into cif-file
PDF-4+ 2023
File Window Help
Open PDF Cards
Preferences
Search
History Results
Composition Graph
SIeve+ Microanalysis
Search
Na2 Si2 O5 - 00-053-1234
File Plots
Export
Temperature Series
2D Structure
SAED Pattern
EBSD Pattern
Ring Pattern
Simulated Profile
Raw Diffraction Data
To Crystallographic Information File (*.cif)...
To Bruker TOPAS File (*.str)
To ICDD XML File (*.xml)
Wavelength: Cu Kα1 1.54056 Å
Raw diffraction data
Neutron diffraction
Fixed Slit Intensity
Electron diffraction
Periodic Table
Formula/Name
Classifications
Crystallography
Modulated
Diffraction
Physical Properties
Reference
Comments
Search Reset Tab
2θ (°) d (Å) I h k l *
12.854 6.88136 4 1 1 0
14.665 6.03539 11 0 2 0
18.095 4.89834 11 1 2 0
19.735 4.49483 1 0 1 1
21.119 4.20329 5 1 0 -1
21.175 4.19230 1 2 0 0
21.220 4.18351 11 1 0 1
22.361 3.97255 15 1 1 -1
22.435 3.95962 100 2 1 0
Intensity
2θ (°)
PDF
Experimental
Physical
Crystal
Structure
Classifications
Cross-references
References
Comments
Status: Primary
Quality Mark: Star
Environment: Ambient
Temperature: 298.0 K (Assigned by ICDD editor)
Pressure: -
Phase: δ
Chemical Formula: Na2 Si2 O5
Structural Formula: -
Empirical Formula: Na2 O5 Si2
Refined Formula: -
Weight %: Na25.24 O43.92 Si30.84
Atomic %: Na22.22 O55.56 Si22.22
Compound Name: Sodium Silicate
Mineral Name: - IMA No: -
Zeolite Name: -
Alternate Name: δ-Na2 Si2 O5
CAS Number: -
Entry Date: 09/01/2003
Modification Date: - Modifications: -


PDF-4+ 2023
File Window Help
Open PDF Cards
Preferences
Search
History Results
Composition Graph
SIeve+ Microanalysis
Search
Na2 Si2 O5 - 00-053-1234
File Plots
Export
Print
Temperature Series
Toolbox
Property Sheet
2D Structure
3D Structure
Bonds
SAED Pattern
EBSD Pattern
Ring Pattern
Simulated Profile
Raw Diffraction Data
X-ray diffraction
Wavelength: Cu Kα1 1.54056 Å
Simulated profile (Exp-based)
Raw diffraction data
Neutron diffraction
Fixed Slit Intensity
Electron diffraction
Periodic Table
Formula/Name
Classifications
Crystallography
Modulated
Diffraction
Physical Properties
Reference
Comments
Search Reset Tab
2θ (°) d (Å) I h k l *
12.854 6.88136 4 1 1 0
14.665 6.03539 11 0 2 0
18.095 4.89834 11 1 2 0
19.735 4.49483 1 0 1 1
21.119 4.20329 5 1 0 -1
21.175 4.19230 1 2 0 0
21.220 4.18351 11 1 0 1
22.361 3.97255 15 1 1 -1
22.435 3.95962 100 2 1 0
Intensity
2θ (°)
PDF
Experimental
Physical
Crystal
Structure
Classifications
Cross-references
References
Comments
ICDD Calculated Parameters
Space Group: P21/n (14)
Molecular Weight: 182.15 g/mol
Crystal Data
a: 8.382 Å α: 90.00° Volume: 490.31 Å³ c/a: 0.578
b: 12.073 Å β: 90.30° Z: 4.00 a/b: 0.694
c: 7.345 Å γ: 90.00° c/b: 0.401
Reduced Cell
a: 8.382 Å α: 90.00° Volume: 490.31 Å³
b: 8.382 Å
c: 12.073 Å
Check crystal information during search