



Sieve+ Introduction

- Sieve+ is a Plug-In module integrated in the PDF-4 products. Sieve+ is licensed separately at an additional cost except for the PDF-4/Organics database. Sieve+ will activate for a free 30-day trial period or until the product is registered. A license for Sieve+ may be purchased along with a PDF-4 license or following the free 30-day trial period.
- Sieve+ accepts user data and searches the ICDD reference databases (PDF-4+, Organics, and Minerals) for comparison. There are several hundred thousand entries for both PDF-4+ and Organic databases. Therefore, various methods, especially the **newly implemented features and improvements** listed below are used to ensure efficient searches to obtain the accurate matches.
 - ❖ New Similarity Index with normalized R index
 - ❖ New data processing menu for background subtraction, Ka2 stripping, smoothing, and peak finding
 - ❖ New Matches Filter with Common Filters of Primary Patterns or Mineral Related or Common Phases
 - ❖ Instant display of overlapping input and reference patterns
- The matched results depend on the criteria and methods specified. This tutorial demonstrates the available methods and the operational procedures of Sieve+.

Sieve+ Purpose

Sieve+ will identify patterns of various X-ray powder diffraction (XRPD) data files:

- 1. Single phase XRPD patterns**
- 2. Multi-phase XRPD patterns**
- 3. Data file containing only XRPD peaks (*.xml)**
- 4. Raw instrumental and/or converted data file formats:**

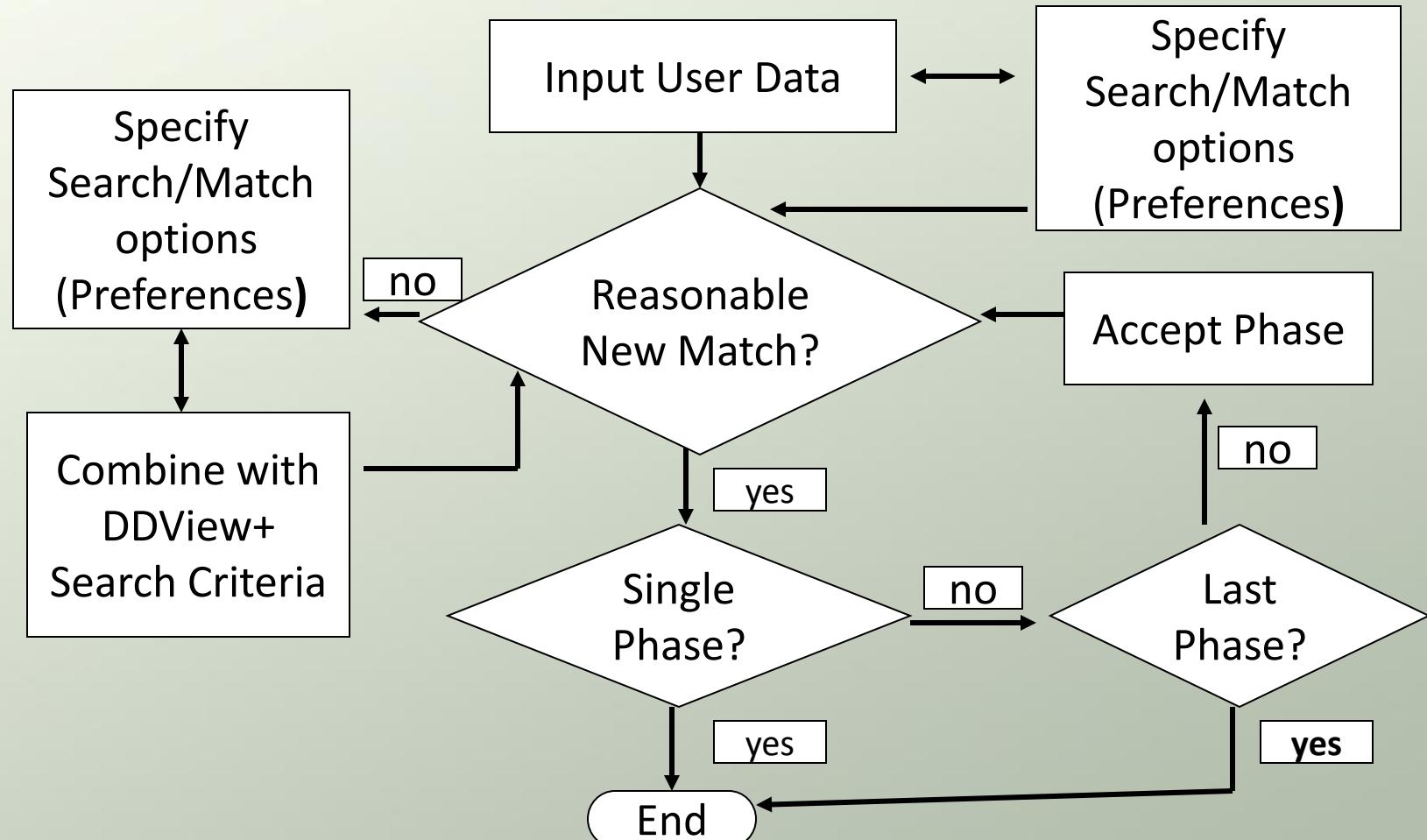
ICDD	(*.csv, *.prn, *. *.pd3)
CIF	(*.cif)
X-Y	(*.xrd)
GSAS	(*.gsas, *.gss, *.gsa, *.raw, *.dat)
Bruker	(*.uxd)
MDI	(*.mdi)
PANalytical	(*.xrdml, *.udf)
Scintag	(*.ard)
Sietronics	(*.cpi)

Sieve+ Methods

There are different search methods and match criteria used to get accurate results. They include:

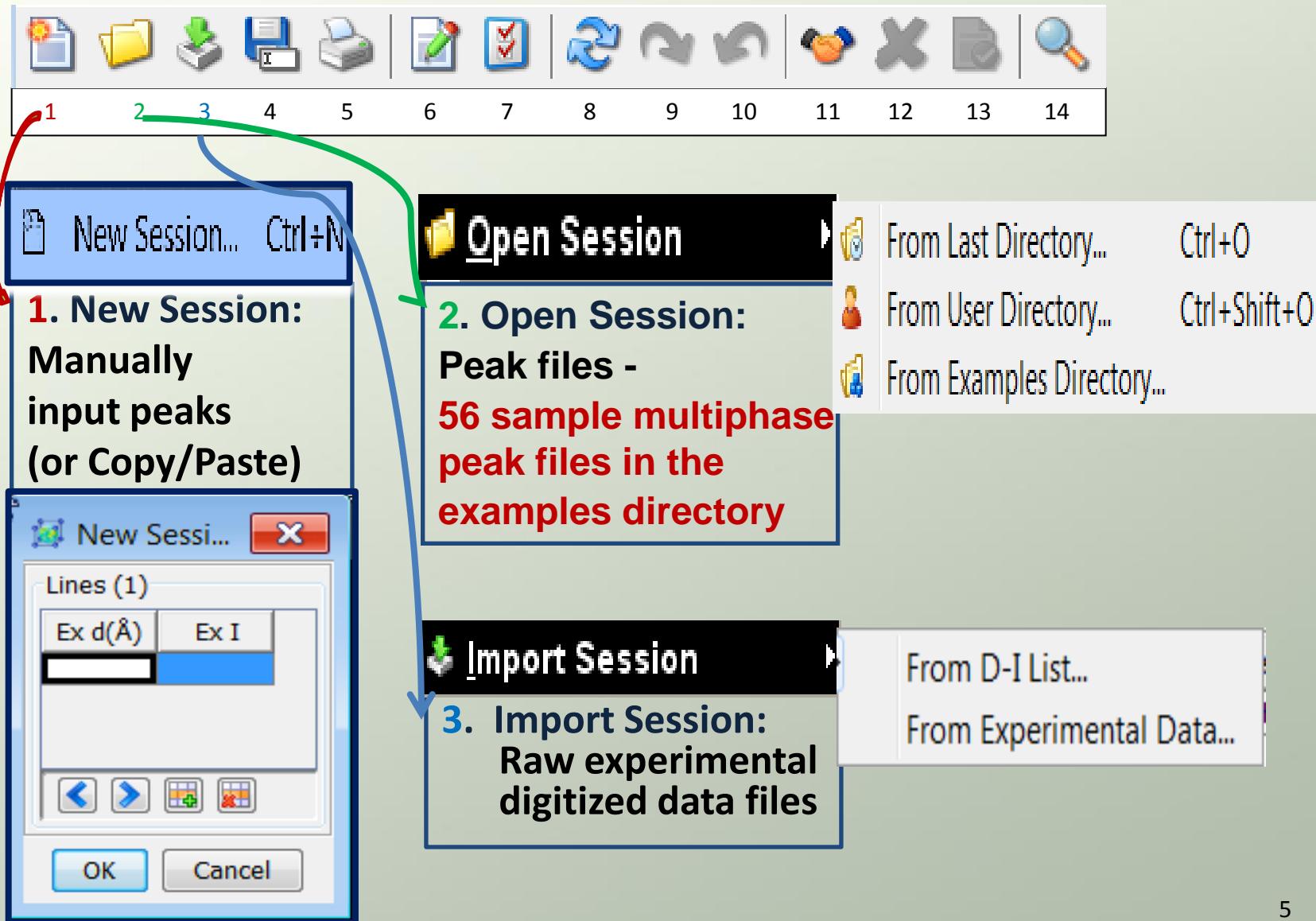
1. Hanawalt with the option of 3 rotations – This uses the strongest line for the search. The rotation involves up to the 3 strongest lines
2. Fink with the option of 8 rotations – This uses the longest of the 8 strongest lines for the search. The rotation involves up to the 8 strongest lines.
3. Eight largest d-spacings with the option of 8 rotations – This method uses the largest of the 8 longest lines for the search.
4. Search window and Match window are options for user to specify the error margin.
5. Weighted GOM, Pattern GOM, and Similarity Index are quantities used to rank the matched reference patterns.
6. Data file import processing options – Manually add/delete points or use Cubic Spline function for background subtraction; Add diffraction peaks; Strip Ka2 peaks prior to file import.

SIeve+ Search/Match Procedure



Sieve+ User Data Input

Frequently Used Icons



The image shows the Sieve+ software interface with the 'File' menu open. The menu items are:

- New Session... Ctrl+N
- Open Session
 - From Last Directory... Ctrl+O
 - From User Directory... Ctrl+Shift+O
 - From Examples Directory...
- Import Session
 - From D-I List...
 - From Experimental Data...

A red circle highlights the 'New Session...' icon (icon 1). A green arrow points from the 'Open Session' icon (icon 2) to its submenu. A blue arrow points from the 'Import Session' icon (icon 3) to its submenu.

1. New Session:
Manually
input peaks
(or Copy/Paste)

2. Open Session:
Peak files -
56 sample multiphase peak files in the examples directory

3. Import Session:
Raw experimental
digitized data files

New Sess...

Lines (1)

Ex d(Å) Ex I

OK Cancel

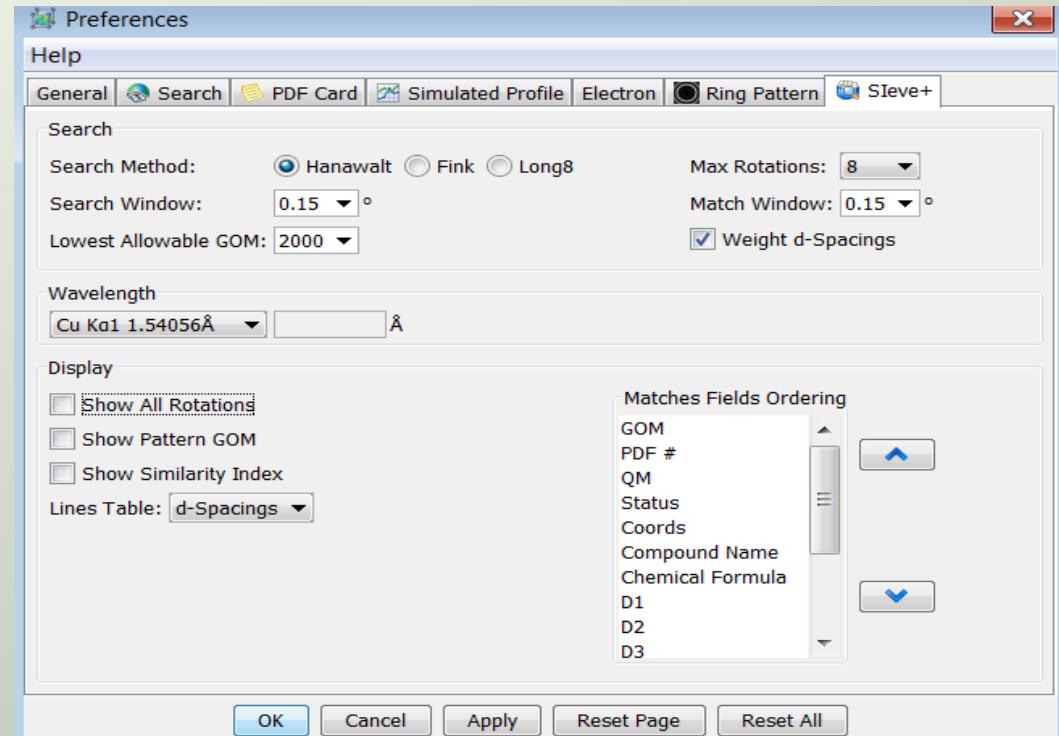
Sieve+ Miscellaneous Options

Frequently Used Icons



7. Sieve+ Preference: Methods and Criteria window

- Search/Match error margin
- Wavelength specification
- GOM limit specification
- Hanawalt/Fink/Long8 selection
- Show/Hide All Rotation
- Show/Hide Pattern GOM
- Show/Hide Similarity Index
- D-Spacings/2Theta selection



11. Accept Phase

Comparison between the

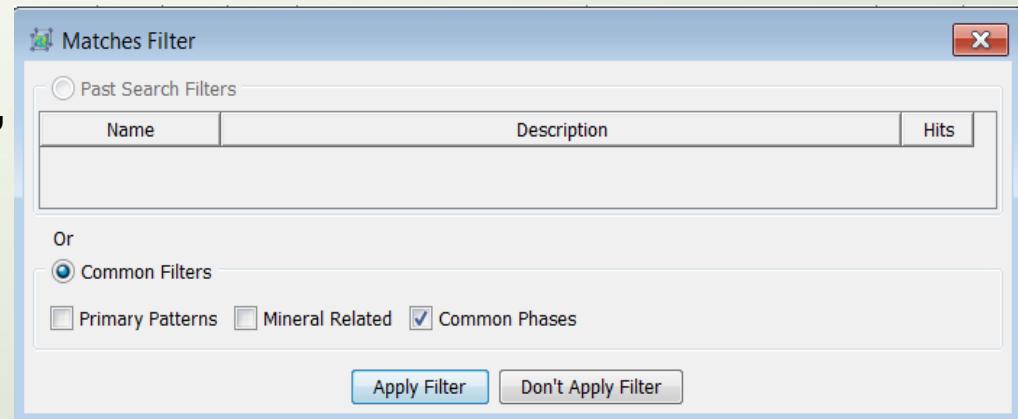
user data and reference data continues after “accepting” the matched phase

Phases (2)		#	PDF #	Compound Name	I Ratio	I %	I/Ic
	1		04-007-9627	Zinc Oxide	1.1	80	5.11
	2		04-005-4213	Aluminum Oxide	0.27	20	1.02

Sieve+ Phases Table – Multiphase Hit List

Matches Filter:

Combine the chemical, physical, and crystallographic property from the previous search with the d-spacings/intensity search results.



Phases (3)

	#	PDF #	Compound Name	I Ratio	I %	I/Ic
	1	✓ 04-007-9627	Zinc Oxide	1.1	49	5.11
	2	✓ 04-005-4213	Aluminum Oxide	0.27	12	1.02
	3	04-002-5299	Calcium Fluoride	0.89	39	3.84

Three matched referenced patterns from the PDF database:

- The mixed phases contain Zinc Oxide, Aluminum Oxide, and Calcium Fluoride
- Sum (intensities) of matched peaks for reference pattern 04-007-9627 / Sum (intensities) of matched peaks for unknown mixed phase = 1.1
- (1.1 / (1.1+0.27+0.89)) * 100 = 49
- I/Ic: reported reference intensity ratio in PDF database for 50/50 weight percent for [Reference Pattern]/Corundum

Sieve+ Lines Table - Phase Comparison

d-spacings/Intensities of Multi-phases and those of reference patterns comparison table:

1st & 2nd columns:
Experimental data.

3rd & 4th columns:
First matched reference pattern data.

5th & 6th columns:
Second matched reference pattern data.

7th & 8th columns:
Third matched reference pattern data.

Diffraction Patterns Lines (41 of 44)

Ex d ↓	Ex I	P1 d	P1 I	P2 d	P2 I	P3 d	P3 I
3.47551	13			3.476710	64		
3.15138	82					3.153050	98
2.81186	58	2.812850	58				
2.60078	42	2.602000	45				
2.54880	23			2.548790	100		
2.47398	100	2.474510	100				
2.37763	9			2.377000	47		
2.08383	24			2.083380	98		
1.93049	89					1.930840	100
1.92175	4						
1.90973	23	1.910090	23				
1.73900	11			1.738350	49		
1.64662	27					1.646630	30
1.62391	35	1.624000	31				
1.60066	23			1.600060	94		
1.47645	30	1.476480	26				
1.40671	6	1.406430	4				
1.40377	8			1.403160	37		
1.37777	26	1.377680	22				
1.37324	14			1.372360	56		
1.36533	10					1.365310	10
1.35777	12	1.357720	10				
1.30105	2	1.301000	2				
1.25308	8					1.252890	9
1.23833	6	1.237250	3	1.238110	16		
1.23352	2			1.233150	8		
1.11489	14					1.114770	15
1.09266	8	1.092470	6				
1.06326	3	1.063160	2				

Sieve+ Case-1

Objective: Search for reference patterns in the PDF database to match mixed phase peaks in a user file

1. File => Open Session =>
From Examples Directory

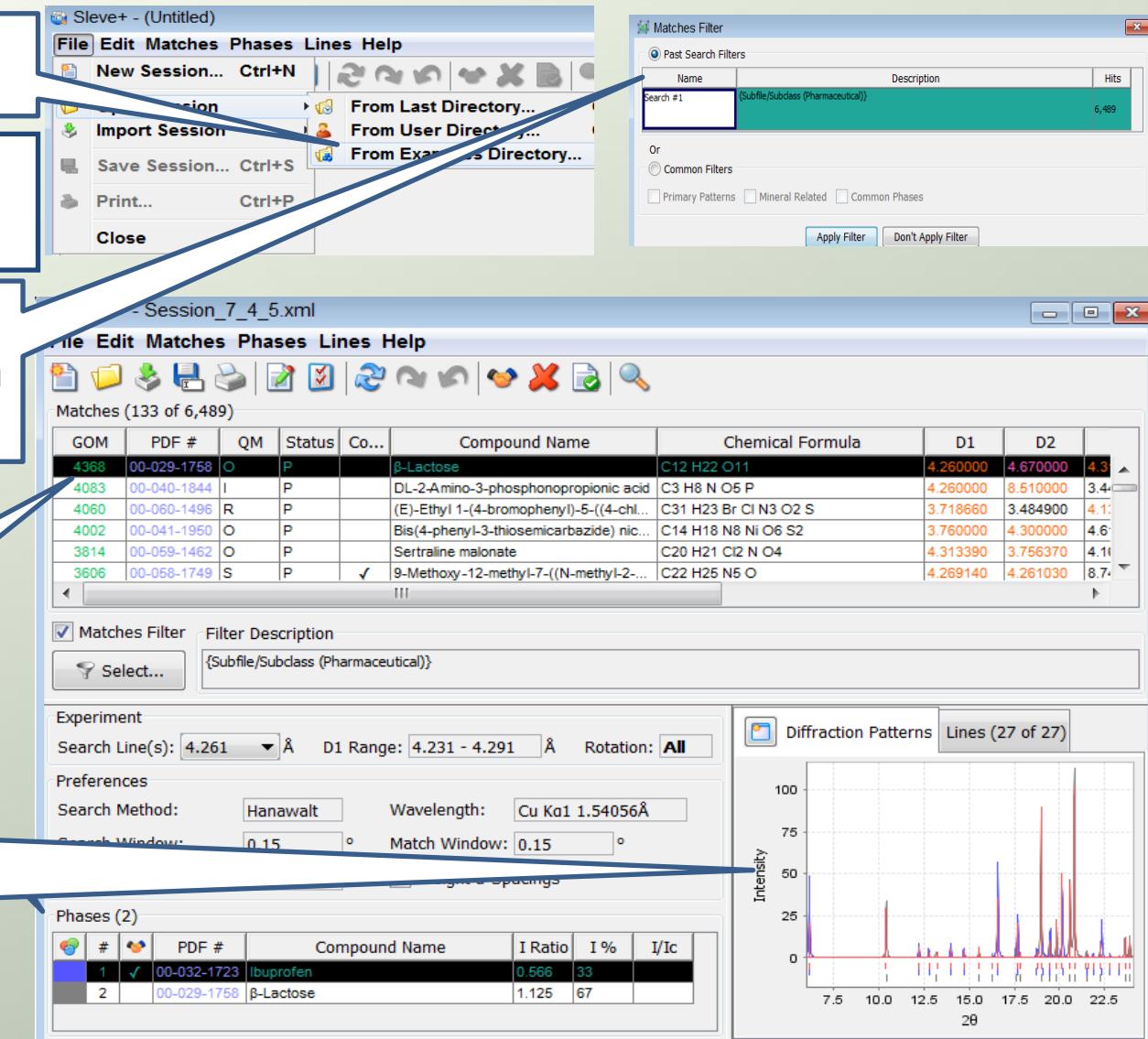
2. Select a peak file:
Session_7_4_5.xml

3. Select Matches Filter
“ICDD Pharmaceutical” from
the previous search results

4. Accept “Ibuprofen”,
continue Searching

5. 2nd matched phase
 β -Lactose with
highest GOM

6. Diffraction Patterns:
unknown and
matched reference
patterns' d-spacings
and intensities



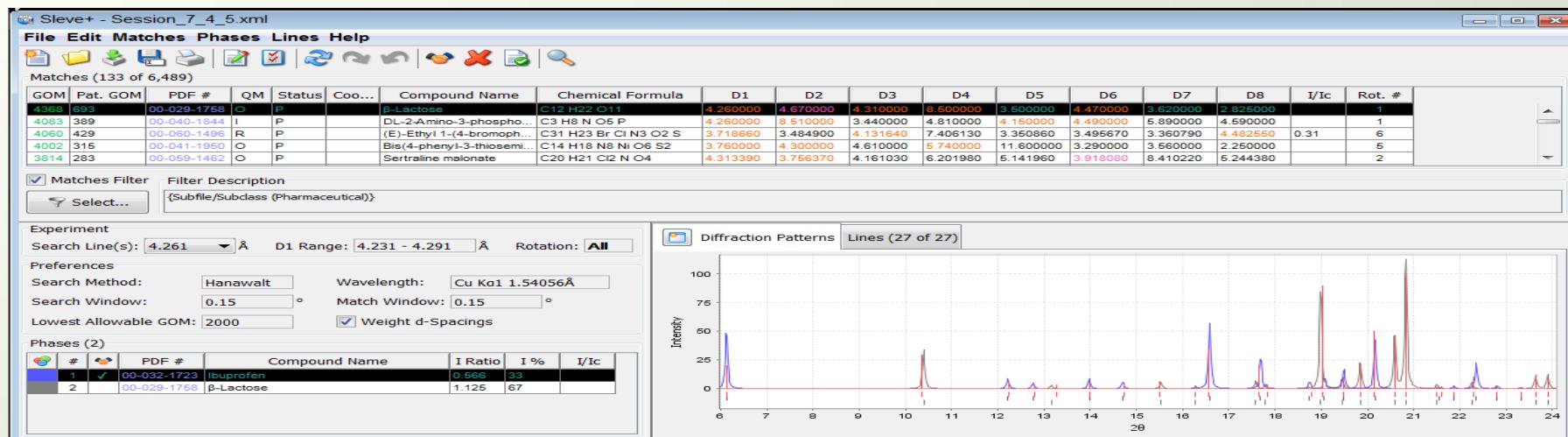
The screenshot shows the Sieve+ software interface with several windows open:

- File Menu:** Shows options like New Session..., From Last Directory..., From User Directory..., and From Examples Directory... (which is highlighted).
- Matches Filter Window:** Displays a table of search filters, with "Search #1 (Subfile/Subclass (Pharmaceutical))" selected.
- Matches Window:** Shows a list of 133 matches from 6,489 results. The first few entries are:

GOM	PDF #	QM	Status	Co...	Compound Name	Chemical Formula	D1	D2	...
4368	00-029-1758	O	P		β -Lactose	C12 H22 O11	4.260000	4.670000	4.3
4083	00-040-1844	I	P		DL-2-Amino-3-phosphonopropionic acid	C3 H8 N O5 P	4.260000	8.510000	3.4
4060	00-060-1496	R	P		(E)-Ethyl 1-(4-bromophenyl)-5-((4-chl...	C31 H23 Br Cl N3 O2 S	3.718660	3.484900	4.1
4002	00-041-1950	O	P		Bis(4-phenyl-3-thiosemicarbazide) nic...	C14 H18 N8 Ni O6 S2	3.760000	4.300000	4.6
3814	00-059-1462	O	P		Serrataline malonate	C20 H21 Cl2 N O4	4.313390	3.756370	4.1
3606	00-058-1749	S	P	✓	9-Methoxy-12-methyl-7-((N-methyl-2-...	C22 H25 N5 O	4.269140	4.261030	8.7
- Diffraction Patterns Window:** Shows Intensity vs. 2θ (degrees) for the unknown pattern (red line) and the reference pattern for Ibuprofen (blue line). The x-axis ranges from 7.5 to 22.5 degrees, and the y-axis ranges from 0 to 100 intensity.
- Phases Window:** Displays the identified phases with their GOM numbers, PDF numbers, compound names, I Ratios, I %, and I/Ic values. It lists Ibuprofen (GOM 1, PDF 00-032-1723, I Ratio 0.566, I % 33, I/Ic 1.0) and β -Lactose (GOM 2, PDF 00-029-1758, I Ratio 1.125, I % 67, I/Ic 1.0).

Sieve+ Case-1

Interpretation of matched results



$$\Delta = \text{window} * d / \tan(\arcsin(\lambda / (2 * d)))$$

A Match: reference d-spacing \leq experimental d-spacing $\pm \Delta$

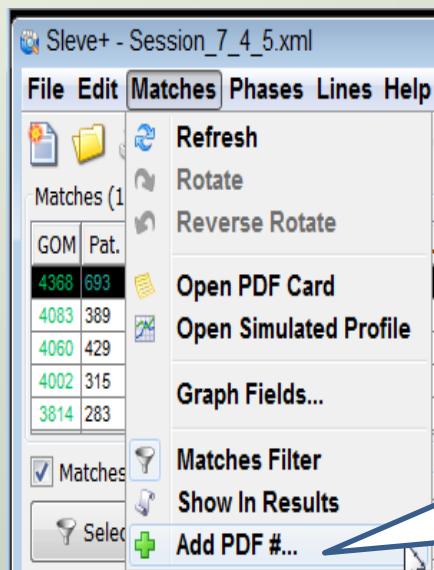
Red: matched lines; **Black:** non-matched lines; **Purple:** overlapped lines

Goodness of Match (GOM):

$$\text{GOM (each line)} = (1 - (\text{line error} / \Delta)) * (1 - (\text{line error} / \Delta)) * 1000$$

$$\begin{aligned} \text{GOM (Final Weighted)} &= (\text{D1 GOM} * 3) + (\text{D2 GOM} * 2) + \\ &\quad (\text{D3 GOM}) + (\text{D4 GOM} * 0.4) + (\text{D5 GOM} * 0.4) + \\ &\quad (\text{D6 GOM} * 0.4) + (\text{D7 GOM} * 0.4) + (\text{D8 GOM} * 0.4) \end{aligned}$$

If a suspected reference pattern is not in the "Matches" table, users can use the new option "Add PDF #" under the "Matches" tab to manually add the pattern to the "Matches" table.



Sieve+ Case-2

Objective: Find matched patterns in the PDF database with the experimental raw data containing three phases of compounds.

1. Import raw experimental data file – a mixture of three phases for search/match

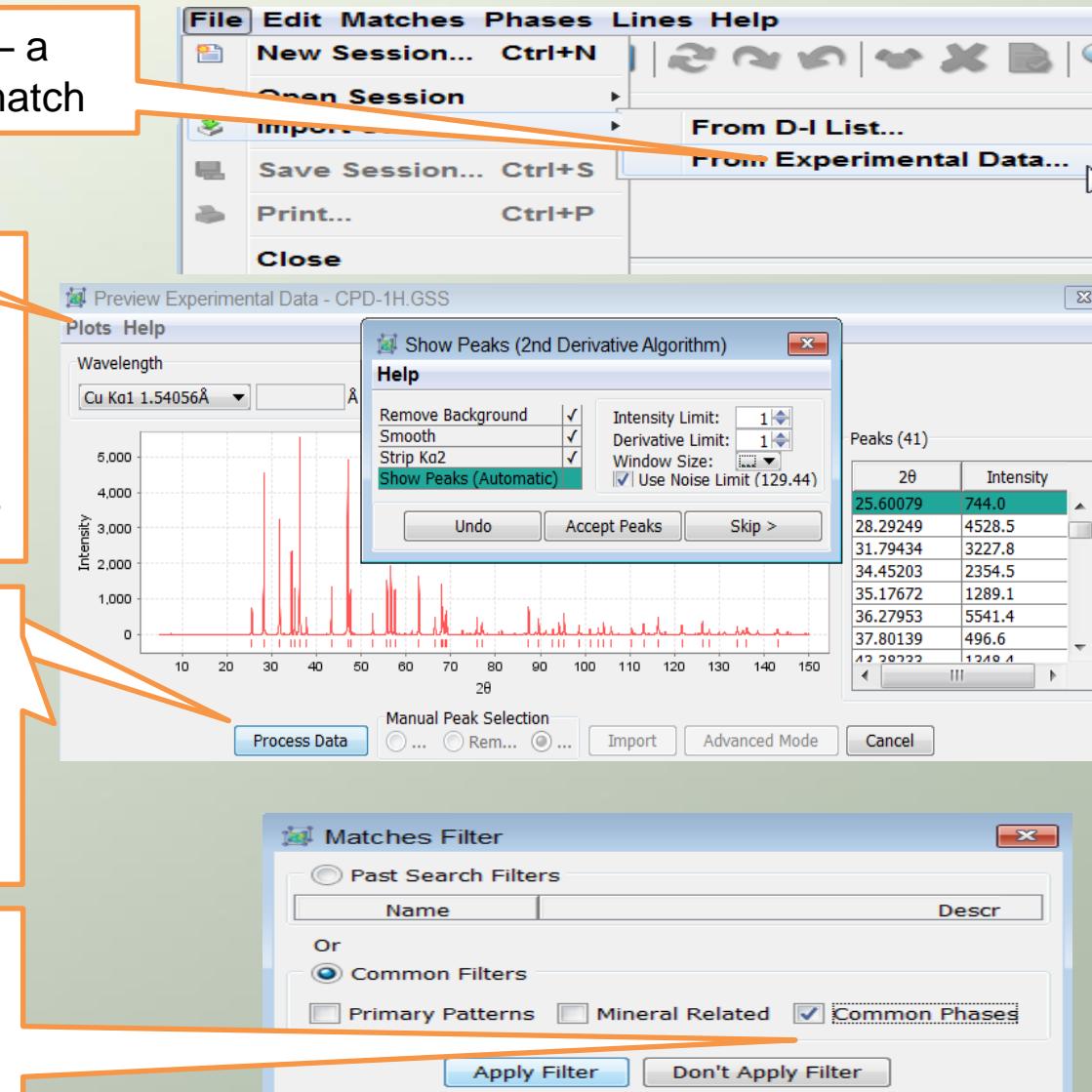
Zero point correction

2. Process Data

- ❖ Background Subtraction
- ❖ Smoothing
- ❖ Strip Ka2 Peaks
- ❖ Show Peaks, Add/Remove Peaks

At the end of data processing, tick marks shown at the bottom of the plot indicate all peaks for the search. Also, a peak table on the right side shows the total number of peaks.

After Importing the data, “Common Phase” of the “Common Filters” was selected to reduce the number of matches.



Sieve+ Case-2

Multiphase Search/Match Results

Matches (67 of 19,489)

GOM	PDF #	QM	S...	Co...	Compound Name	Chemical Formula	D1	D2	D3	D4	D5	D6	D7	D8
7264	04-007-9627	P	A	✓	Zinc Oxide	Zn O	2.474510	2.812850	2.602000	1.624000	1.476480	1.910090	1.377680	1.357720
7264	04-008-7114	P	A	✓	Zinc Oxide	Zn O	2.474510	2.812850	2.602000	1.624000	1.476480	1.910090	1.377680	1.357720
6733	01-070-8072	S	A	✓	Zinc Oxide	Zn O	2.473620	2.811550	2.601500	1.623250	1.476090	1.377150	1.909480	1.357110

Matches Filter

Common Phases

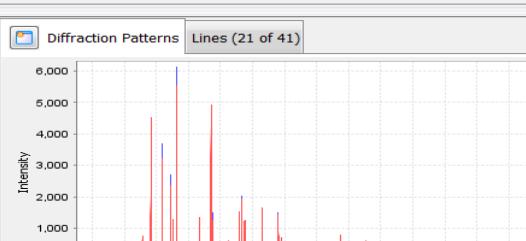
Experiment
Search Line(s): 2.47411 Å D1 Range: 2.464 - 2.484 Å Rotation: 1 of 8

Preferences
Search Method: Hanawalt Wavelength: Cu K α 1 1.54056 Å
Search Window: 0.15 Match Window: 0.15
Lowest Allowable GOM: 2000 Weight d-Spacings

Phases (1)

#	PDF #	Compound Name	I Ratio	I %	I/Ic
1	04-007-9627	Zinc Oxide	1.105	100	5.11

First matched phase
ZnO with highest GOM



Comparison of d-spacings and intensities for the input data and those of all three reference patterns

Matches (38 of 19,489)

GOM	PDF #	QM	S...	Co...	Compound Name	Chemical Formula	D1	D2	D3	D4	D5	D6	D7	D8
6802	04-002-5299	I	A	✓	Calcium Fluoride	Ca F ₂	1.930840	3.153050	1.646630	1.114770	1.366310	1.252890	0.863498	1.051020
6791	04-006-0187	I	A	✓	Calcium Fluoride	Ca F ₂	1.930750	3.152910	1.646550	1.114720	1.365250	1.252840	0.863460	1.050970
6762	00-004-0864	S	A	✓	Calcium Fluoride	Ca F ₂	1.931000	3.153000	1.647000	1.115000	1.366000	1.253000	0.863700	1.051200

Matches Filter

Common Phases

Experiment
Search Line(s): 1.93063 Å D1 Range: 1.925 - 1.936 Å Rotation: 1 of 8

Preferences
Search Method: Hanawalt Wavelength: Cu K α 1 1.54056 Å
Search Window: 0.15 Match Window: 0.15
Lowest Allowable GOM: 2000 Weight d-Spacings

Phases (2)

#	PDF #	Compound Name	I Ratio	I %	I/Ic
1	✓ 04-007-9627	Zinc Oxide	1.105	55	5.11
2	04-002-5299	Calcium Fluoride	0.887	45	3.84

2nd matched phase CaF₂

Matches (36 of 19,489)

GOM	PDF #	QM	S...	Co...	Compound Name	Chemical Formula	D1	D2	D3	D4	D5
5346	01-089-7716	S	A	✓	Aluminum Oxide	Al ₂ O ₃	2.085190	2.550680	1.601280	3.479670	1.373660
5319	00-042-1468	S	D	✓	Aluminum Oxide	Al ₂ O ₃	2.085000	2.551000	1.601400	3.480000	1.373800
5170	00-005-0712	I	A	✓	Aluminum Oxide	Al ₂ O ₃	2.085000	2.552000	1.601000	3.479000	1.374000

Matches Filter

Common Phases

Experiment
Search Line(s): 2.08407 Å D1 Range: 2.077 - 2.091 Å Rotation: 1 of 8

Preferences
Search Method: Hanawalt Wavelength: Cu K α 1 1.54056 Å
Search Window: 0.15 Match Window: 0.15
Lowest Allowable GOM: 2000 Weight d-Spacings

Phases (3)

#	PDF #	Compound Name	I Ratio	I %	I/Ic
1	✓ 04-007-9627	Zinc Oxide	1.105	49	5.11
2	✓ 04-002-5299	Calcium Fluoride	0.887	39	3.84
3	01-089-7716	Aluminum Oxide	0.255	11	0.99

3rd matched phase Al₂O₃

