SIeve Introduction

- SIeve is a Plug-In module to the DDView software which is integrated in the PDF-2 products. SIeve is licensed separately at an additional cost. 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-2 license or following the free 30-day trial period.

- SIeve accepts user data and searches the ICDD reference database PDF-2 for comparison. There are several hundred thousand entries for the PDF-2 database. Therefore, various methods, especially the newly implemented weighted GOM methods, and criteria are used to ensure efficient searches to obtained the accurate matches.

- The matched results depend on the criteria and methods specified. This tutorial demonstrates the available methods and the operational procedure 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:**

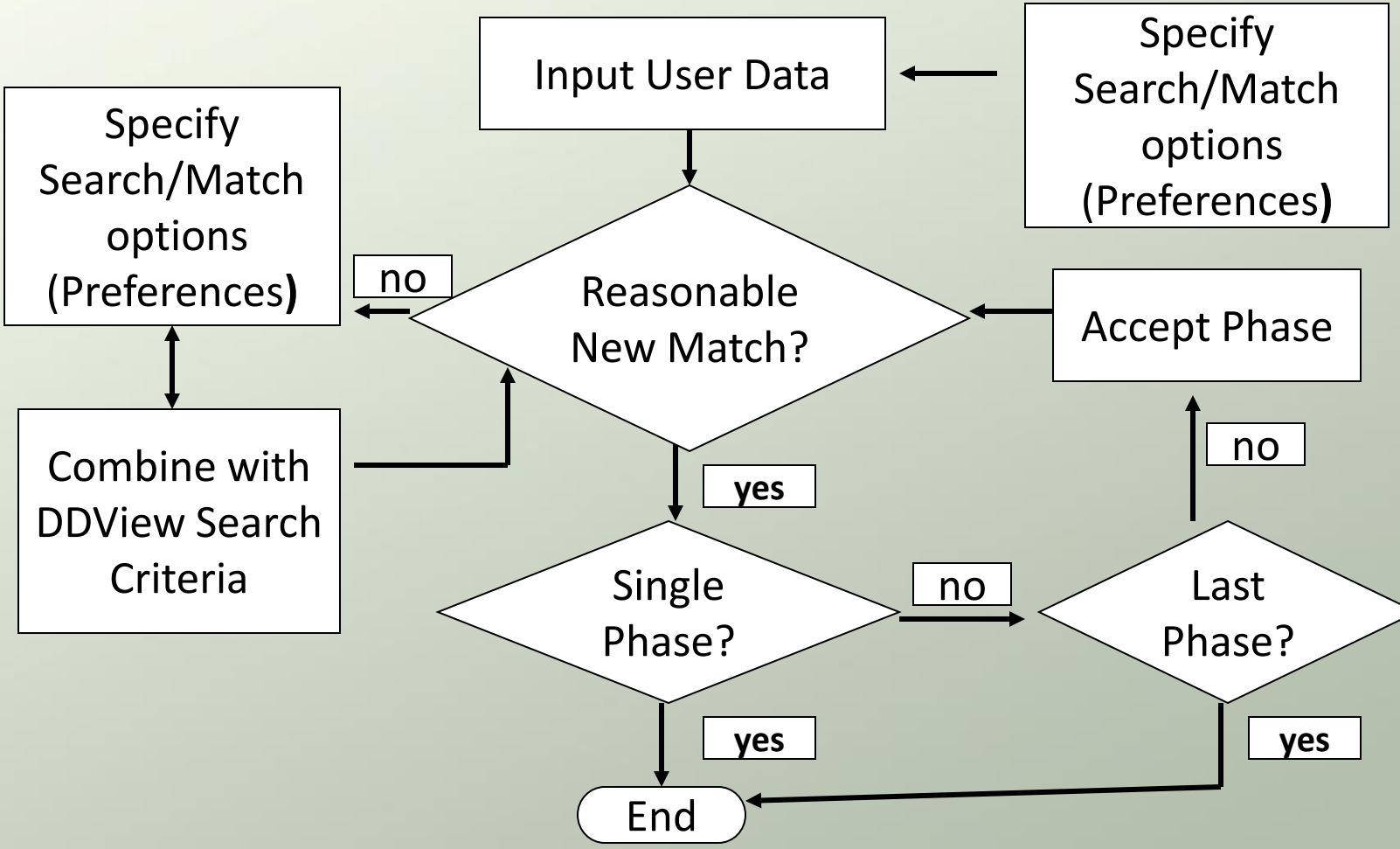
CIF	**(*.cif)**
X-Y	**(*.xrd)**
GSAS	**(*.gsas, *.gss, *.gsa, *.raw, *.dat)**
Bruker	**(*.uxd)**
MDI	**(*.mdi)**
PANalytical	**(*.xrdml, *.udf)**
Scintag	**(*.ard)**
Sietronics	**(*.cpi)**
ICDD text	**(*.csv, *.prn, *.pd3)**

SIeve Methods

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

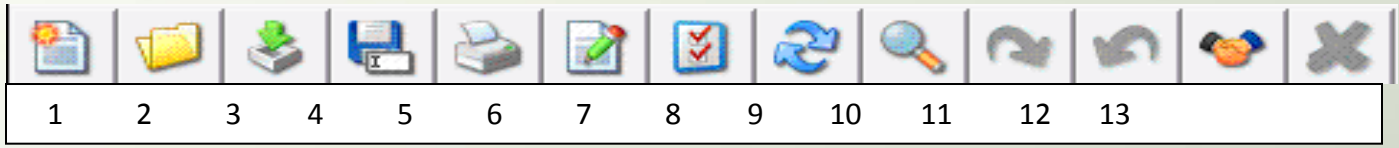
1. Hanawalt with the option of 3 rotations – This uses the strongest line of for search. The rotation involves up to 3 strongest lines
2. Fink with the option of 8 rotations – This uses the longest of the 8 strongest lines for search. The rotation involves up to 8 strongest lines.
3. Eight largest d-spacings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

SIeve Search/Match Procedure



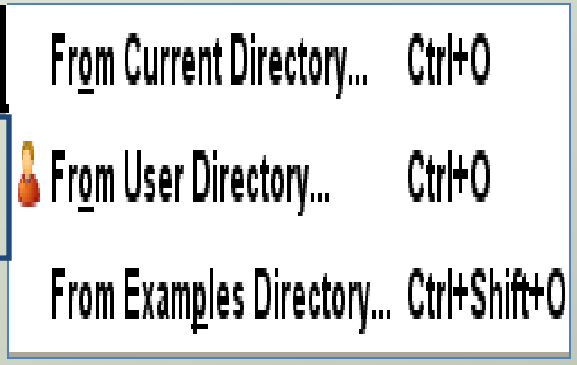
SIeve User Data Input

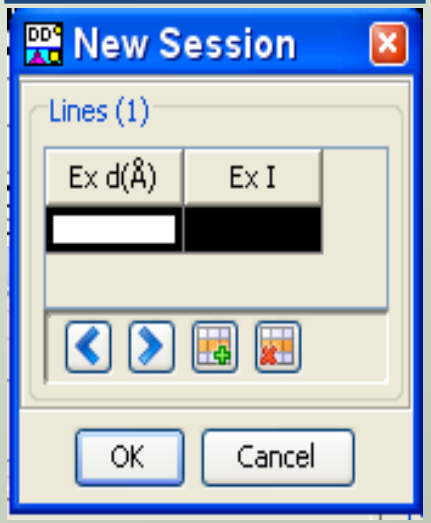
Frequently Used Icons



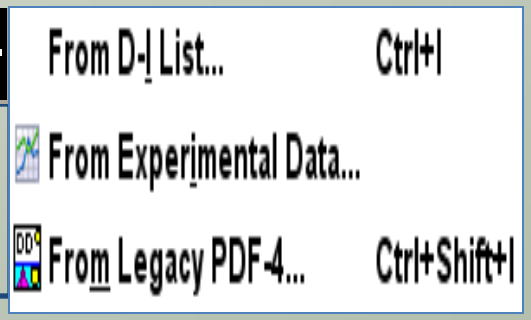
1. New Session: Manually input peaks (or Copy/Past)

2. Open Session: Peak files



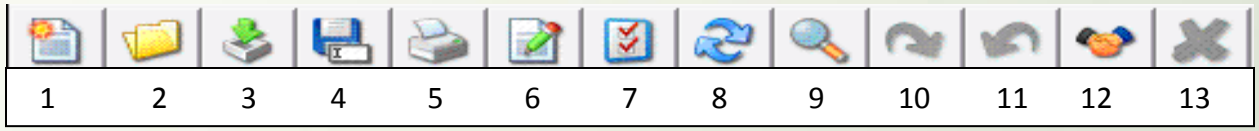


3. Import Session: Raw experimental digitized data files



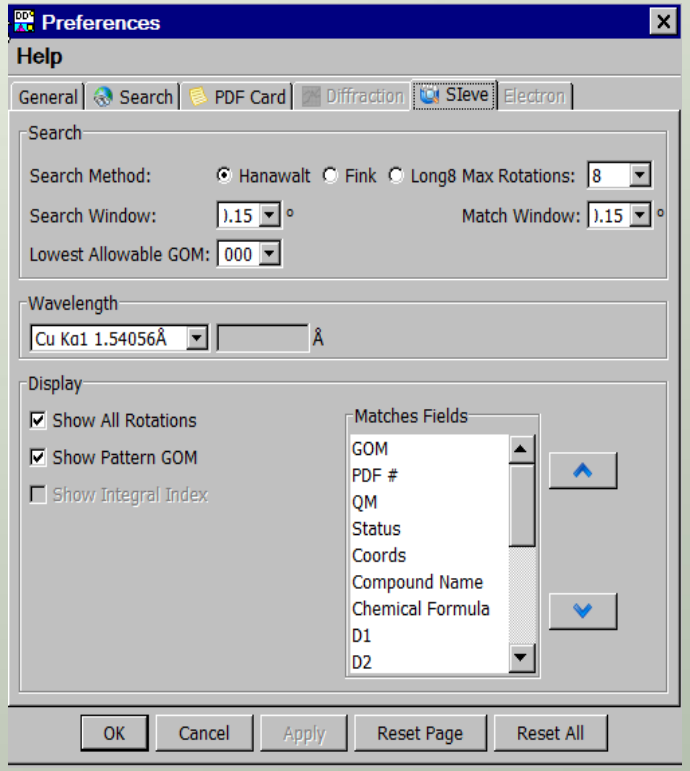
SIeve Miscellaneous Options

Frequently Used Icons



7. SIeve Preference:
Methods and Criteria window-

- **Search/Match error margin**
- **Wavelength specification**
- **GOM limit specification**
- **Hanawalt/Fink /Long8 with rotation specification**
- **New option for viewing the "Matches Fields" in preferred order**
- **New option to display/hide "Pattern GOM" and "Rotations**

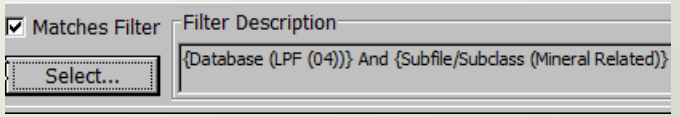


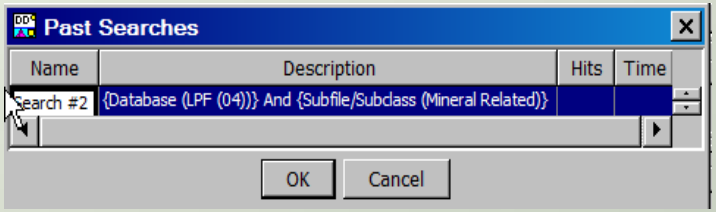
12. Accept Phase
Comparison between the user data and reference data continues after "accepting" the matched phase

#	Accepted	PDF #	Compound Name	Int. Ratio	Int. %	I/Ic	Time
1	✓	00-029-1758	β-Lactose	1.125	67		8.3s
2		00-032-1723	Ibuprofen	0.566	33		8s

SIeve Phases Table – Multiphase Hit List

Matches Filter:
Combine the chemical, physical, crystallographic property search results from DDView with the d-spacings/intensity search results.





Phases (3)

# ▲	Accepted	PDF #	Compound Name	Int. Ratio	Int. %	I/Ic	Time
1	√	04-003-3353	Silicon	0.771	40	4.55	0.2s
2	√	00-043-1484	Aluminum Oxide	0.21	11	0.98	2.1s
3		04-002-1862	Nickel	0.943	49	7.43	0s

Three matched referenced patterns from the PDF database:

- **The mixed phases contain Silicon, Aluminum Oxide, and Nickel**
- **Sum(intensities) of matched peaks for reference pattern #04-003-3353/ Sum (intensities) of matched peaks for unknown mixed phase = 0.771**
- **(0.771 /(0.771+0.21+0.943)) * 100 = 40**
- **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

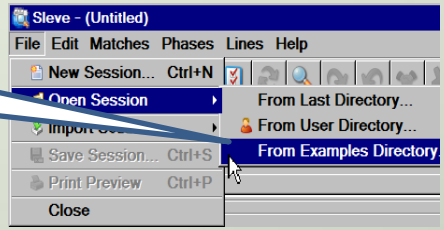
Lines (21 of 24)

Ex d... ▼	Ex I	P1 d(Å)	P1 I	P2 d(Å)	P2 I	P3 d(Å)	P3 I
3.47947	13	3.480000	72				
3.13573	80			3.135500	100		
2.55169	18	2.551000	98				
2.38044	9	2.380000	44				
2.25215	7						
2.08601	20	2.086000	100				
2.03429	100					2.034000	100
1.91942	41			1.920100	55		
1.76156	31					1.762000	42
1.73973	9	1.740100	48				
1.63698	21			1.637500	30		
1.60094	13	1.601500	96				
1.40412	5	1.404600	38				
1.37322	8	1.373900	57				
1.35581	2			1.357700	6		
1.24586	21			1.245900	11	1.246000	21
1.10886	10			1.108600	12		
1.06296	9					1.062400	20
1.05963	5						
1.04543	4	1.046300	1	1.045200	6		
1.01755	3	1.017700	2			1.017200	7
0.91804	8	0.918100	3	0.918000	7		
0.91587	4						
0.90790	3	0.907900	13				

SIeve Case-1

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

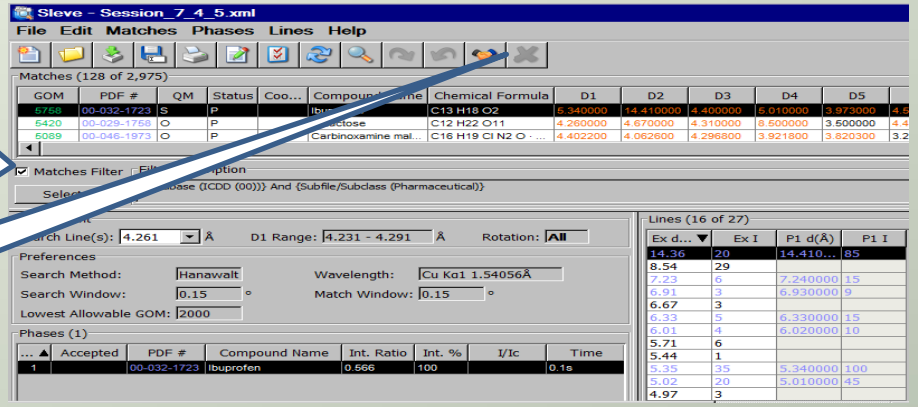
1. File => Open Session => From Eamples Directory



2. Select a peak file: Session_7_4_5.xml

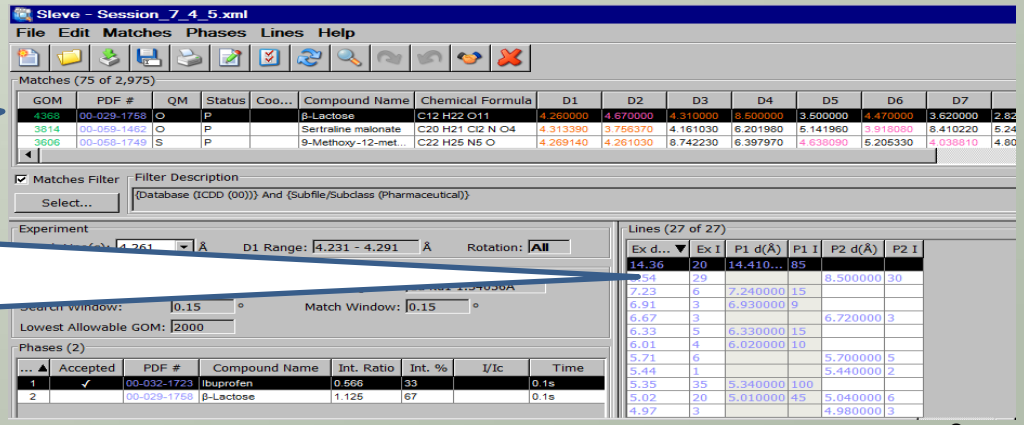
3. Select Matches Filter "ICDD Pharmaceutical" from the DDView search results

4. Accept "Ibuprofen" , continue Searching



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

6. Lines Table: unknown and matched reference patterns' d-spacings and intensities



SIeve Case-1

Interpretation of matched results

Matches (128 of 2,975)

GOM	PDF #	QM	Status	Coo...	Compound Name	Chemical Formula	D1	D2	D3	D4	D5	D6	D7	D8	I/Ic	Rot. #
5758	00-032-1723	S	P		Ibuprofen	C13 H18 O2	5.340000	14.410000	4.400000	5.010000	3.973000	4.550000	7.240000	6.330000		5
5420	00-029-1758	O	P		β-Lactose	C12 H22 O11	4.260000	4.670000	4.310000	8.500000	3.500000	4.470000	3.620000	2.825000		1
5089	00-046-1973	O	P		Carbinoxamine mal...	C16 H19 Cl N2 O · ...	4.402200	4.062600	4.296800	3.921800	3.820300	3.200900	3.341600	3.509200		3
5000	00-001-0374	O	D		α-D-Glucose	C6 H12 O6	4.310000	4.720000	3.160000	2.480000	2.250000	6.080000	5.240000	3.510000		4
5000	00-003-0224	O	D		Thymol	C10 H14 O	4.310000	4.720000	3.490000	3.690000	3.340000	2.830000	2.260000	2.070000		4

Δ = window * d / tan(arcsin(λ / (2 * d)))

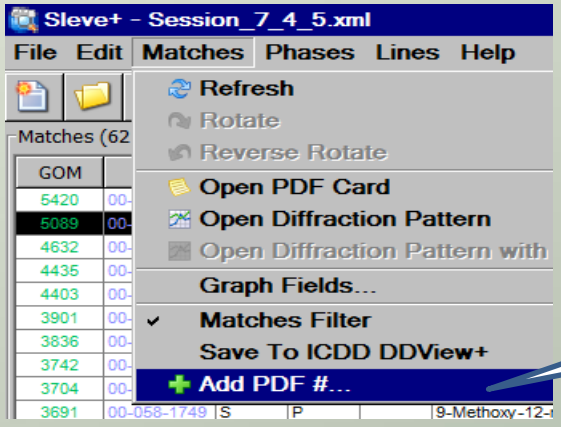
A Match: reference d-spacing <= experimental d-spacing +/- Δ

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

Goodness of Match (GOM):

GOM (each line) = **(** 1 - (line error / Δ) **)** * **(** 1 - (line error / Δ) **)** * 1000

GOM (Final Weighted) = (D1 GOM * 3) + (D2 GOM * 2) +
(D3 GOM) + (D4 GOM * 0.4) + (D5 GOM * 0.4) +
(D6 GOM * 0.4) + (D7 GOM * 0.4) + (D8 GOM * 0.4)

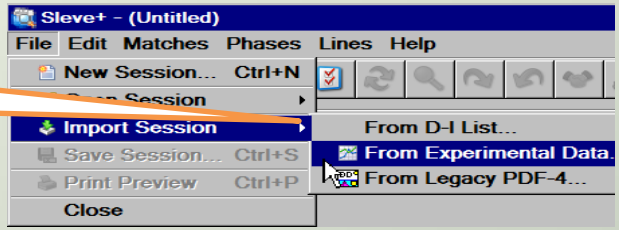


If the suspected reference pattern is not in the “Matches” table, users can use the new option “Add PDF# “ under the “Matches” tab to manually add a pattern to the “Matches” table.

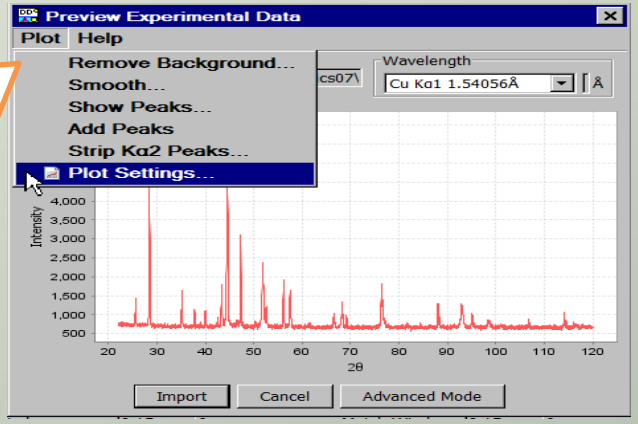
SIeve Case-2 (Auto-Dectect)

Objective: Find matched patterns in the PDF database with the experimental raw data containing three phases of compounds commonly used as XRPD experimental standards .

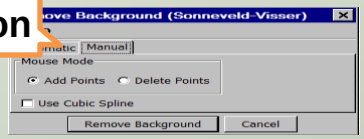
1. Import raw experimental data file “TreePhases.UDF” for search/match

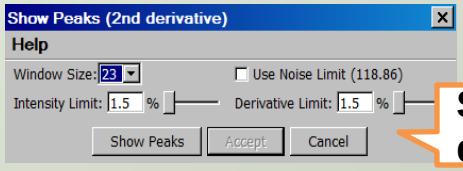


2. Data reduction
Background Subtraction (Automatic, Manual), Smoothing (Savitzky-Golay), Show Peaks, Add Peaks, Strip Ka2 Peaks, Plot Settings (Zero point correction)



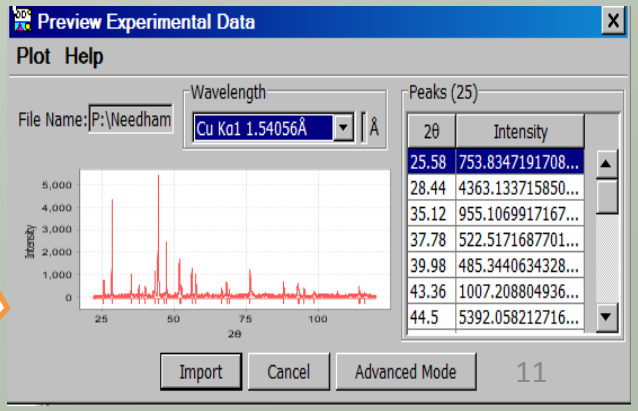
Manual background subtraction





Show Peaks 2nd derivatives parameters

At the end of Data Reduction
Tick marks shown at the bottom of the plot indicate all peaks for search. Also, a peak table on the right side shows the total number of peaks. An alternative data file import method (Advanced mode) is shown on the next slide).



SIeve Case-2

Advanced experimental data input

1. Experimental Wavelength (user input)

2. 2 θ Format (user input) Scan rate, Scan range

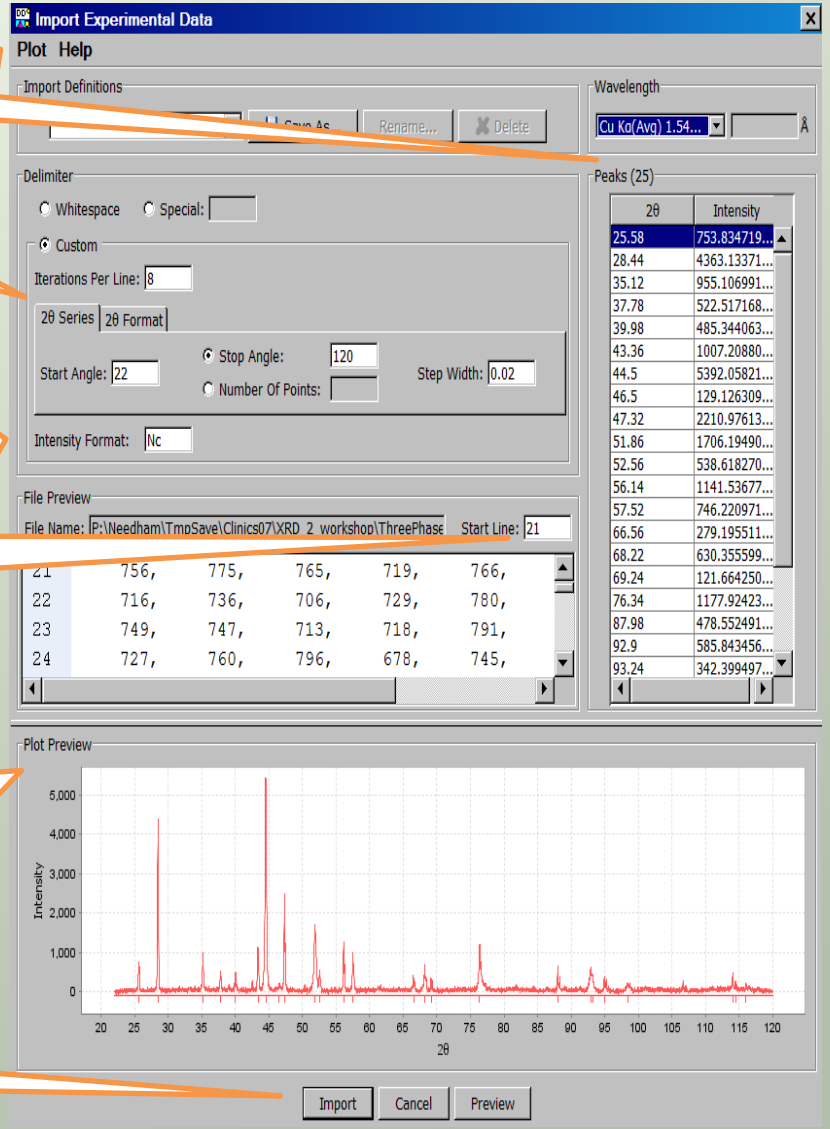
3. Intensity input format (user input, See next slide for all options)

4. Starting line number for the data in the input file (user input)

5. Select “Preview” to view the plot

6.Select “Plot” for data reduction (See the previous Slide)

7. Select “Import” to start Search/Match



SIeve Case-2

Intensity Import format

Input option notations

c	**All characters should be skipped.**
c[#]	**Skip specified numbers (#) of characters.**
n	**All numbers should be skipped.**
t	**All text should be skipped.**
N	**All numbers should be imported.**
N[#]	**Import fixed length data (# = fixed length).**

SIeve Case-2
Multiphase Search/Match