

Example to demonstrate importing an
experiment from an ASCII text file

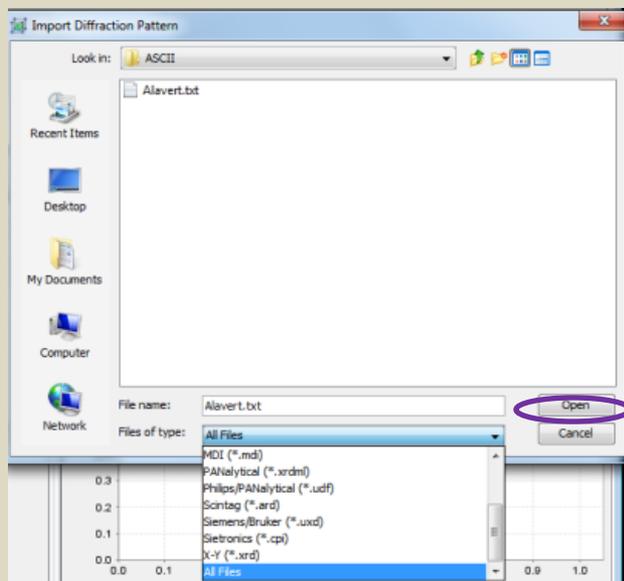
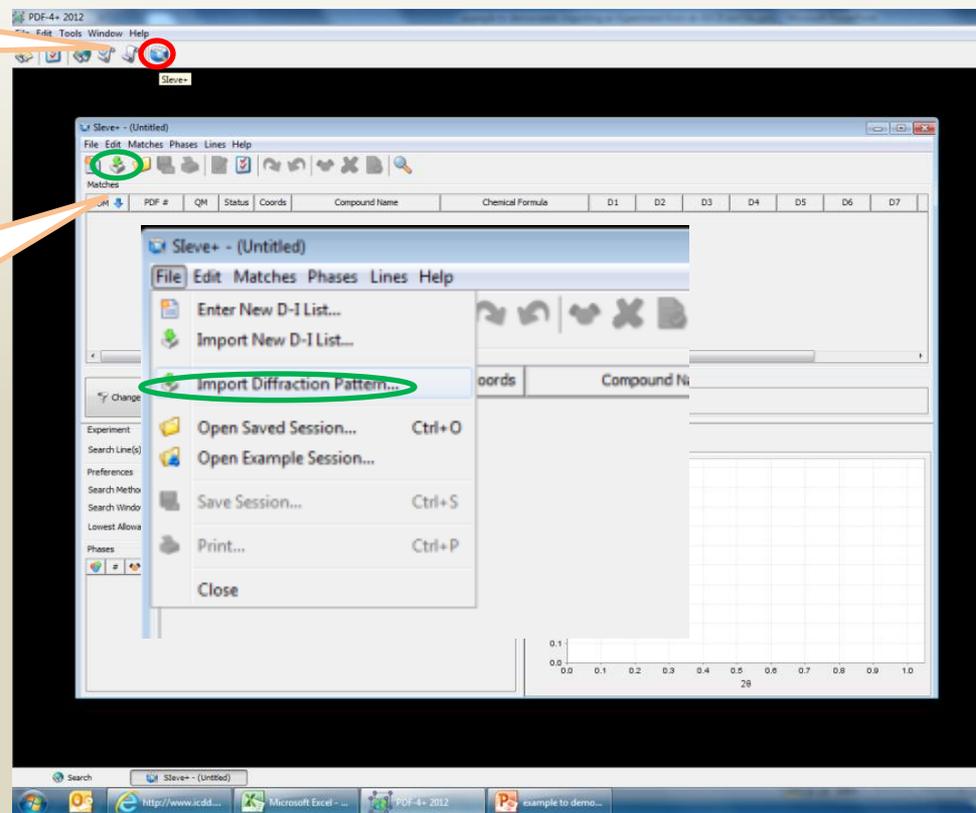
Why need to import data form ASCII text file?

Some data were not saved in commonly used format, or part of the file was damaged, so the file can not be read. In these cases, we can import an experiment data directly from an ASCII text file by the Sieve tool in PDF-4/ PDF-2

Open Sleeve

1. In PDF-4, left click on the icon in the toolbar to open Sleeve

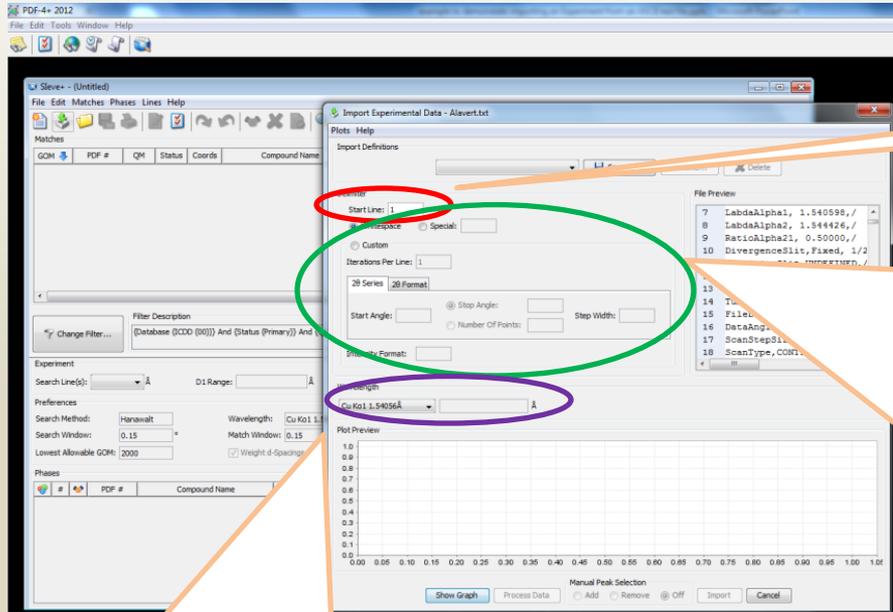
2. Once open Sleeve, left click on import data icon. This function can also be activated from the file menu



3. Select the data file. Most of common formats can be imported directly. If your files are not belonging to these readable formats, you can still change files of type to all files, and then select your data.

Import data

```
## Calibrated wavelength = 0.413891
## Normalization factor = 7.0111
##
## 2theta, intensity, sigma(intensity)
0.500000, 186.990436, 26.470037
0.501000, 163.055531, 24.651342
0.502000, 151.628178, 23.770995
0.503000, 176.085940, 25.609698
0.504000, 175.946894, 25.647889
0.505000, 173.626090, 25.478113
0.506000, 158.407033, 24.361503
0.507000, 167.026713, 25.028063
```



1. Select the start line of the data.

2. If your data contain 2 theta-intensity information as the data I showed up side, you can select white space or type in the character used to separate the column.

If your file contains only the intensity as the file I showed below, you should choose costume, and type in the start angle, step width and stop angle/number of steps. For the intensity format, type in Nc. More explanation about the intensity format option is shown in next slide

3. Select X-ray source. If it is synchrotron radiation, select "other" and then input the wavelength

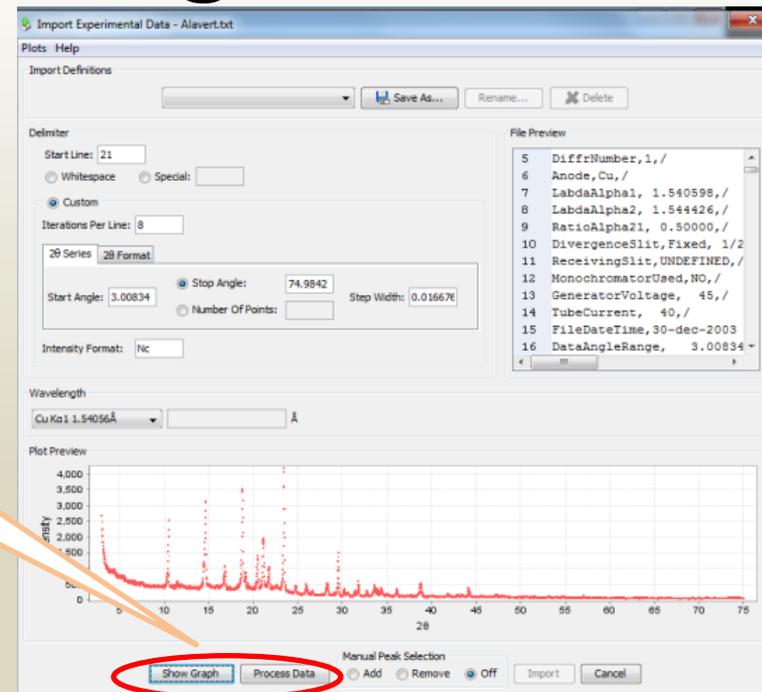
20	RawScan							
21	2669,	2480,	2220,	2263,	2031,	2008,	2049,	1828
22	1828,	1724,	1617,	1607,	1574,	1476,	1501,	1419
23	1374,	1359,	1315,	1278,	1207,	1165,	1287,	1194
24	1144,	1108,	1102,	1081,	1078,	1069,	1108,	1039
25	984,	1069,	1009,	1019,	1001,	1081,	1023,	1054
26	990,	1021,	892,	966,	1001,	981,	930,	886
27	939,	934,	940,	976,	876,	958,	959,	958
28	932,	948,	952,	943,	865,	957,	938,	928

Input option notations

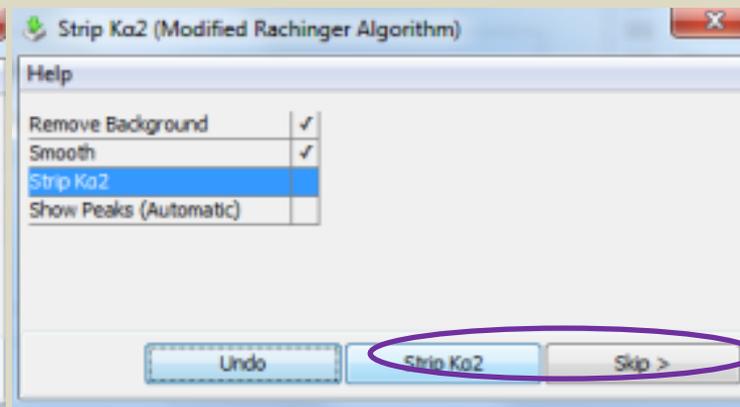
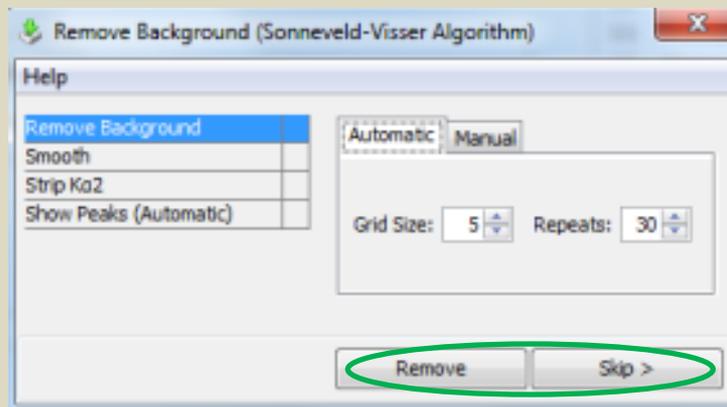
- c All characters should be skipped.
- c[#] Skip specified numbers (#) of characters.
- n All numbers should be skipped.
- t All text should be skipped.
- N All numbers should be imported.
- N[#] Import fixed length data (# = fixed length)

Data processing

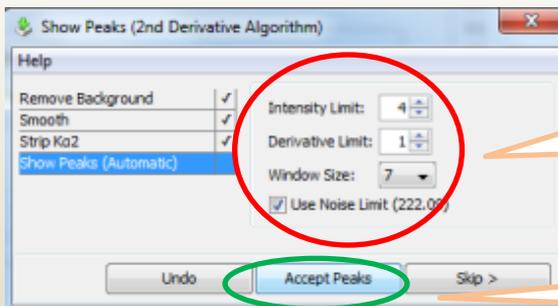
1. Click on show graph gives the figure, and then click on process data to open a new data process window



2. Data process includes background remove, smooth and strip K-alfa2. You can process these steps or skip them if you think they are not necessary.

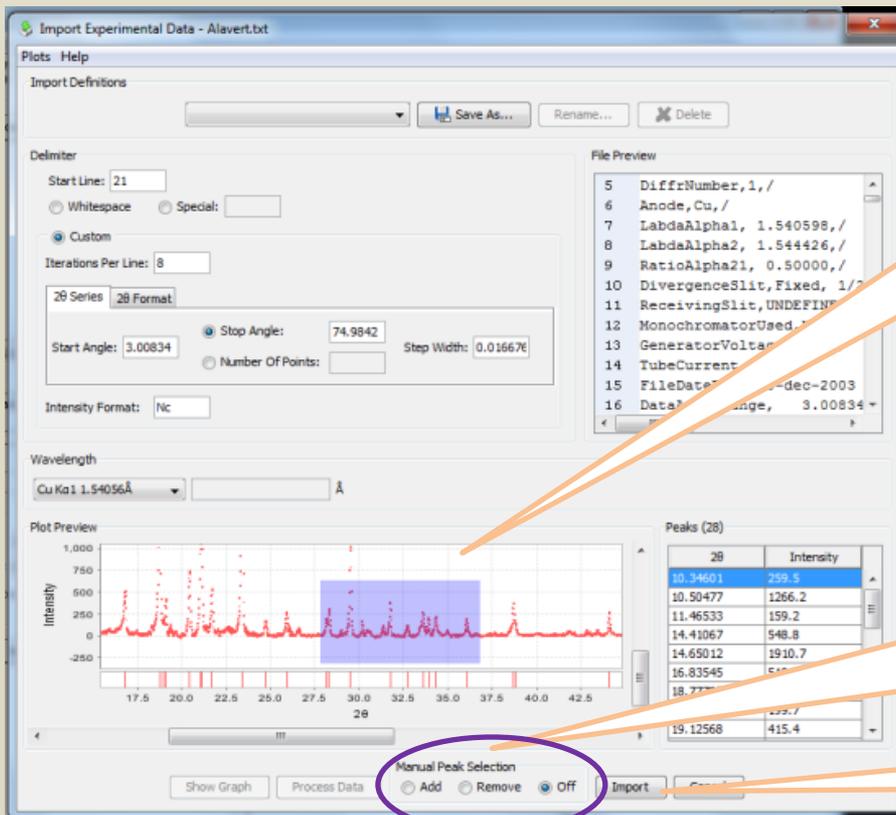


Generate peaks list



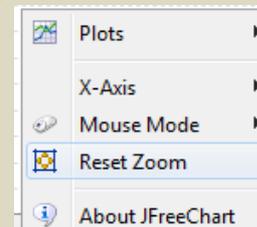
1. Show peaks is the last data process step. Criteria of peak intensity, derivative and window size can be manually set

2. Click accept peaks to create I/d list



Tip: Hold left and drag to zoom in the figure

Tip: Right click on the figure to open the menu for zoom reset



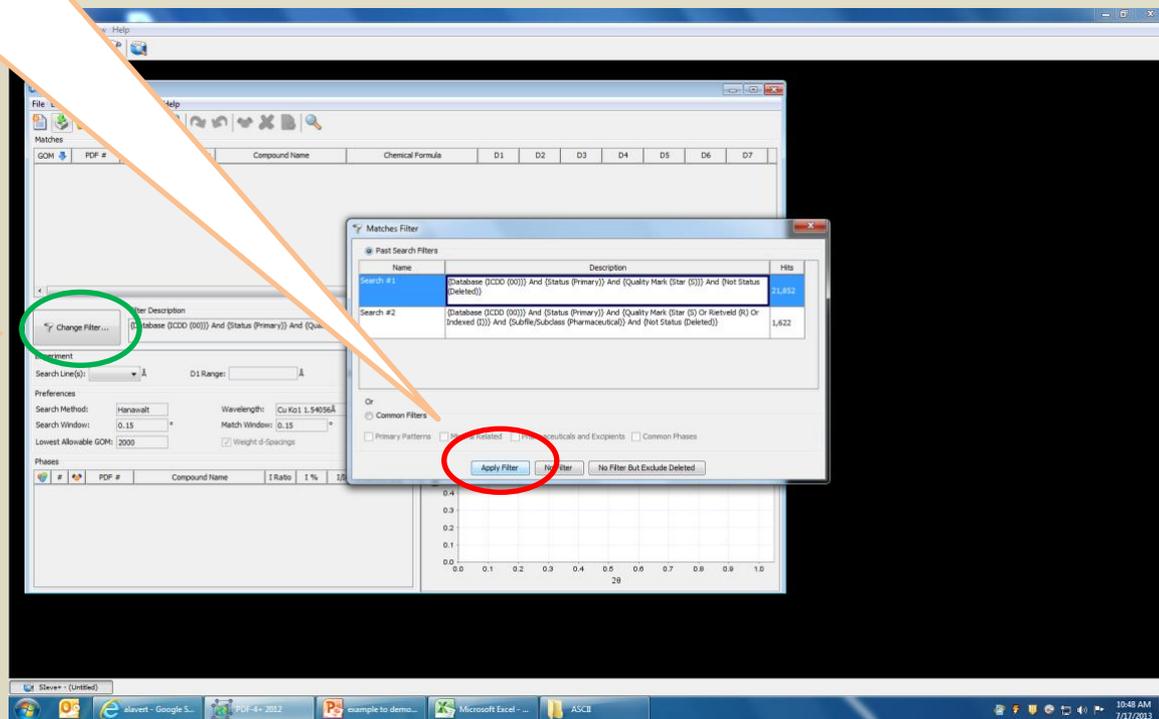
3. Click on add/remove and then click on the figure to manually add/remove the peaks into/from the list

4. Click import to start the search match

Search match

1. To start search match, select the filter and then click apply filter

2. Click change filter to another filter for better result. For more information about setting filters, please check other tutorials.



The screenshot displays the ICDD software interface. A 'Matches Filter' dialog box is open, showing a table of search filters. The 'Apply Filter' button is circled in red. The 'Change Filter...' button in the main window is circled in green. The 'Matches' table in the background shows the following data:

GO#	PDF #	Compound Name	Chemical Formula	D1	D2	D3	D4	D5	D6	D7

The 'Matches Filter' dialog box contains the following table:

Name	Description	Hits
Search #1	[Database (ICDD (00)) And (Status (Primary)) And (Quality Mark (Star (5))) And (Not Status (Deleted))]	11,2812
Search #2	[Database (ICDD (00)) And (Status (Primary)) And (Quality Mark (Star (5) Or Retrieval (R) Or Indexed (I)) And (Subtype/Subclass (Pharmaceutical)) And (Not Status (Deleted))]	1,632

The 'Matches Filter' dialog box also includes options for 'Or', 'Common Filters', 'Primary Patterns', 'Phases', 'Pharmaceuticals and Excipients', and 'Common Phases'. The 'Apply Filter' button is circled in red.