Sort, Order and Graph Data

Sort and Order

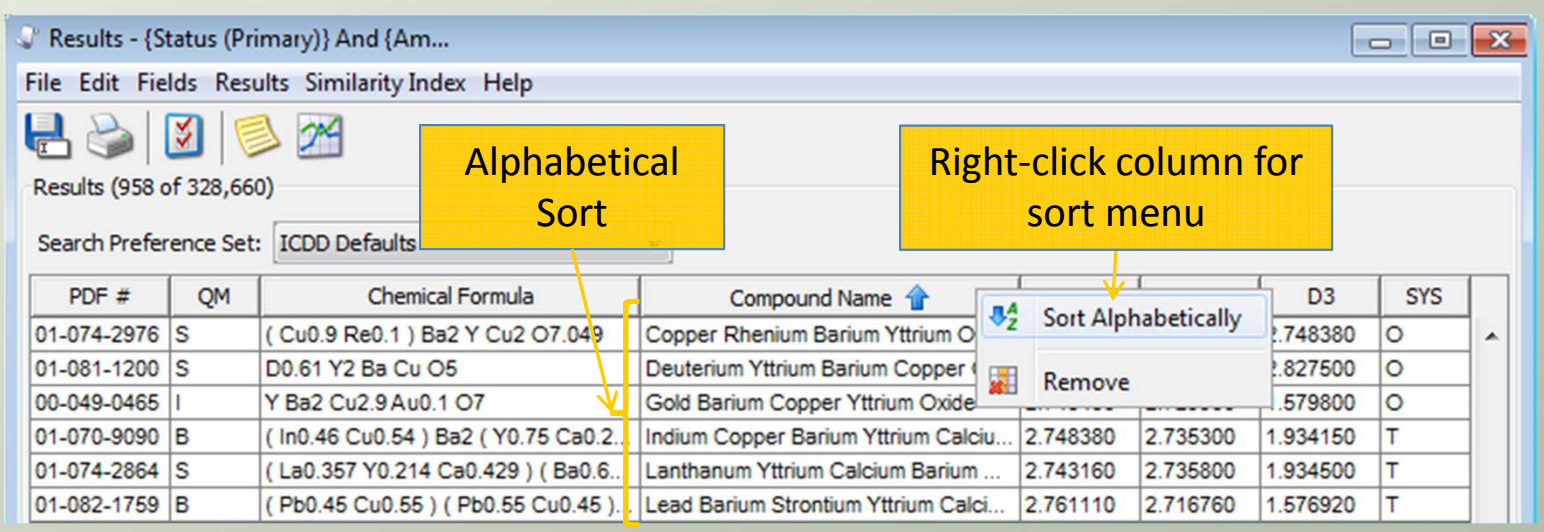
- What?
  - Sorting is the ability to order the PDF data retrieved from the search results.
- Why?
  - To organize the data.
  - To find relevant data faster and easier.
- How?
  - Use the Results table.

Results Table

- The Results table can be sorted on any display field.
- Depending on the display field sorted, there are different types of sorting available:
  - Alphabetical Sort
  - Numerical Sort
  - Special Order Sort
  - Alphabetical Formula Index Sort

Alphabetical Sort

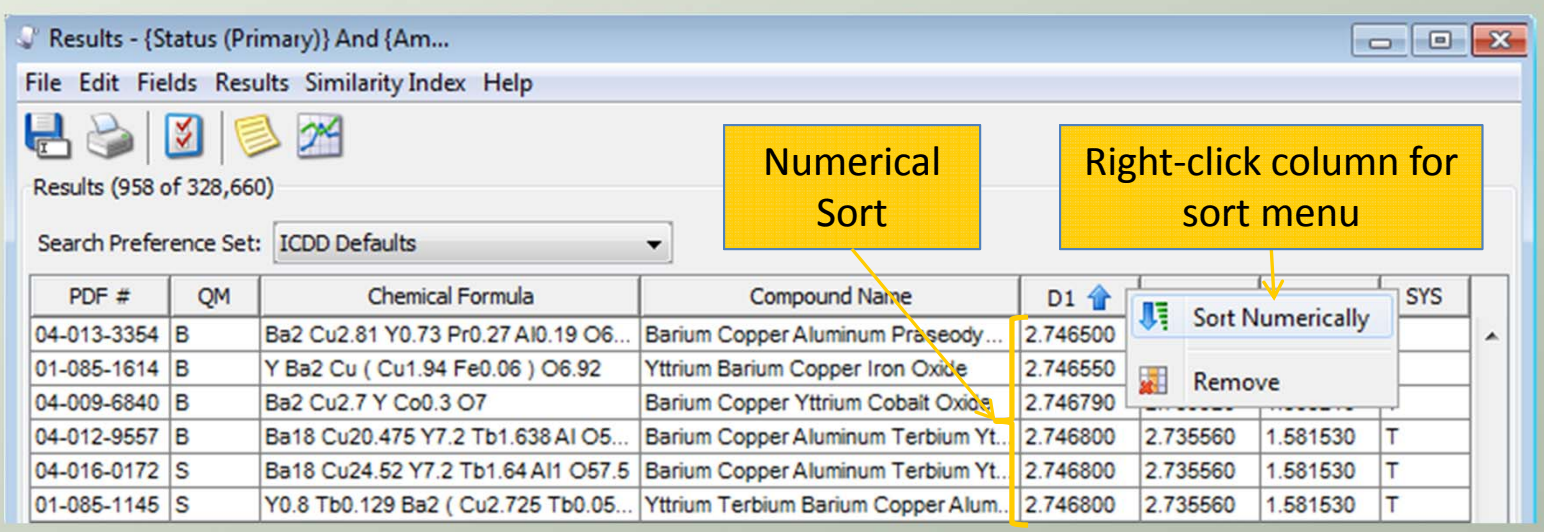
- The Alphabetical Sort will sort a text-based column alphabetically from A - Z.
- This can be performed by:
  - Left-clicking a text-based sort column (e.g., Compound Name).
  - Or middle-clicking a *Special Order* Sort column (e.g., QM).
  - Or right-clicking a text-based sort column and selecting *Sort Alphabetically*.
- Sorting on a *Special Order* Sort column will override the *Special Order* Sort.
- Sorting on a column twice will perform a descending sort from Z – A.



Sorted by Compound Name

Numerical Sort

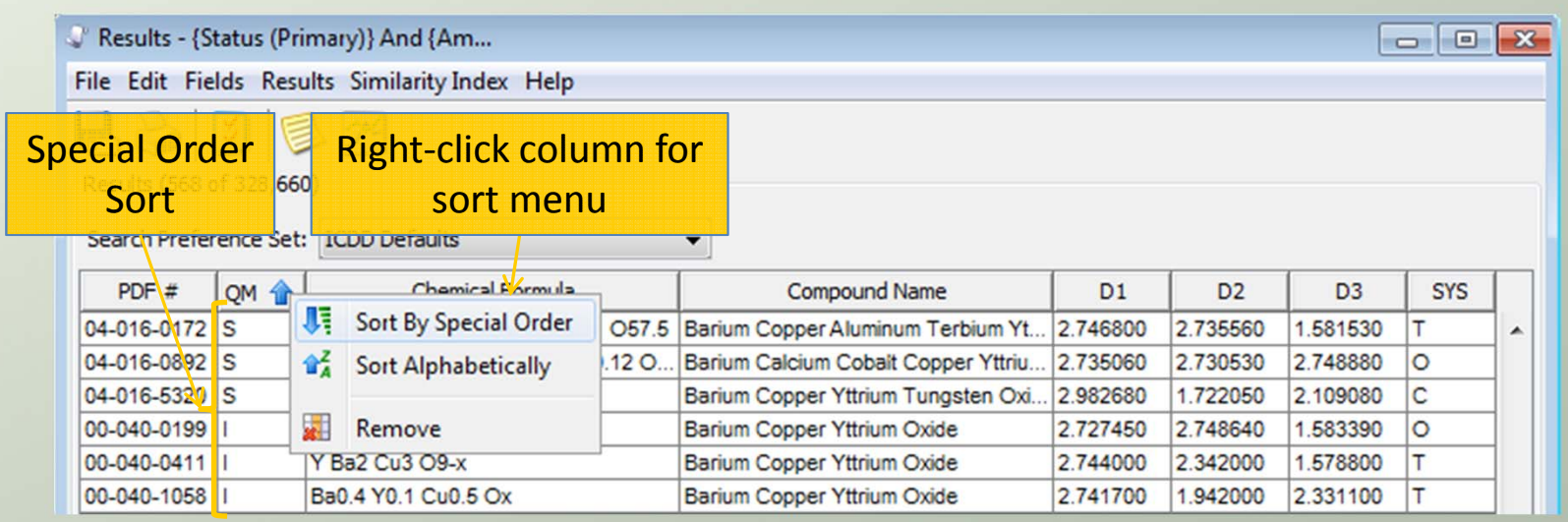
- The *Numerical Sort* will sort a numerical column from 0 – 999…
- This can be performed by:
  - Left-clicking a numerical sort column (e.g., D1).
  - Or right-clicking a numerical sort column and selecting *Sort Numerically*.
- Sorting on a column twice will perform a descending sort from 999… – 0.



Sorted by D1 (Strongest line)

Special Order Sort

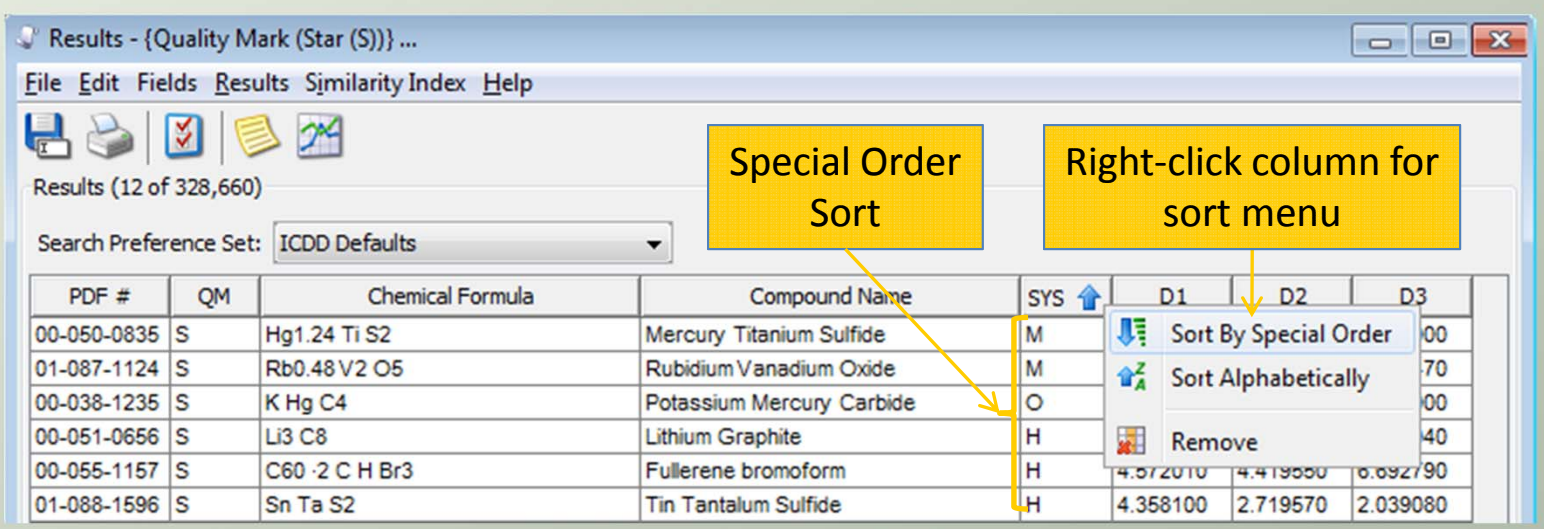
- The *Special Order Sort* will sort a text-based column using an ordering specific to that column. The *Special Order Sort* columns are:
- PDF # (Powder Diffraction File Number)
  - This first orders the PDF #'s by database code: 00 (ICDD), 04 (LPF), 03 (NIST), 02 (CSD), 01 (ICSD).
  - This then orders the PDF #'s by descending set and card number (xx-###-####).
- QM (Quality Mark)
  - Ascending: S (Star), R (Rietveld), I (Indexed), C (Calculated), B (Blank), O (Low-Precision), P (Prototyping), H (Hypothetical), G (Good), M (Minimal Acceptable)
  - Descending: M (Minimal Acceptable), G (Good), H (Hypothetical), P (Prototyping), O (Low-Precision), B (Blank), C (Calculated), I (Indexed), R (Rietveld), S (Star)



Sorted by QM (Quality Mark) showing S (Star) patterns first, as they are of the highest quality.

Special Order Sort

- SYS (Crystal System)
  - Ascending: A (Anorthic), M (Monoclinic), O (Orthorhombic), T (Tetragonal), H (Hexagonal), R (Rhombohedral), C (Cubic), X (Unassigned)
  - Descending: C (Cubic), R (Rhombohedral), H (Hexagonal), T (Tetragonal), O (Orthorhombic), M (Monoclinic), A (Anorthic), X (Unassigned)
- Pearson (Pearson Symbol Code)
  - This first orders by the Crystal Symmetry: a, m, o, t, h, c, ?
  - Secondly, this orders by the Lattice Centering: P, R, C, I, F, ?
  - Thirdly, this orders by the Atomic Count ascending.
- Status
  - Ascending: P (Primary), A (Alternate), D (Deleted)
  - Descending: D (Deleted), A (Alternate), P (Primary)

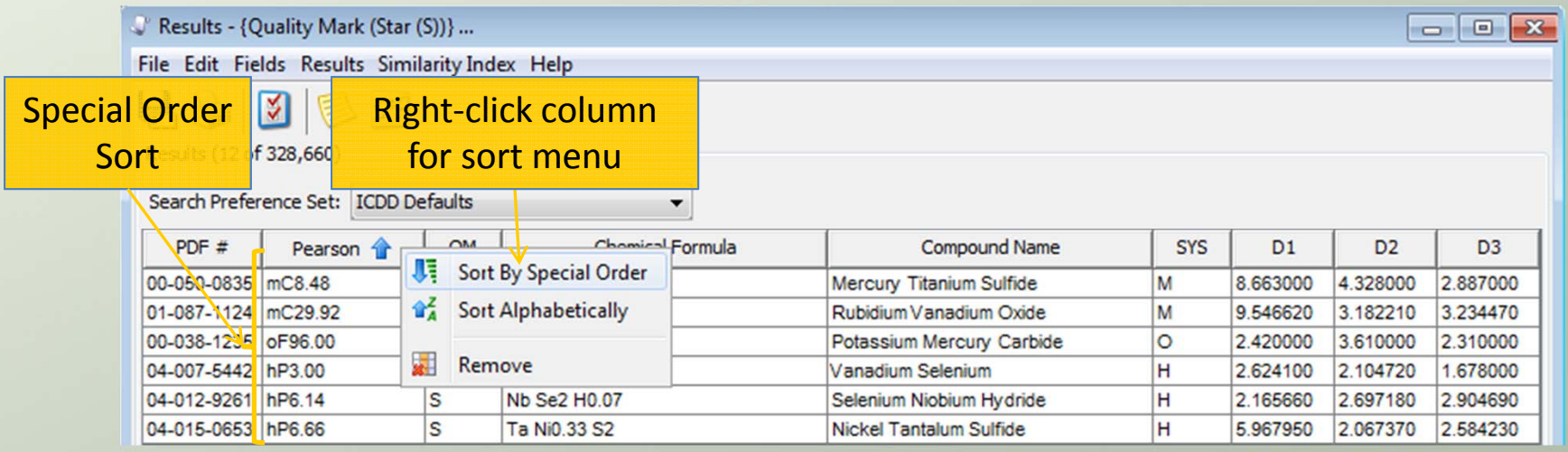


PDF #	QM	Chemical Formula	Compound Name	SYS	D1	D2	D3
00-050-0835	S	Hg1.24 Ti S2	Mercury Titanium Sulfide	M			00
01-087-1124	S	Rb0.48 V2 O5	Rubidium Vanadium Oxide	M			70
00-038-1235	S	K Hg C4	Potassium Mercury Carbide	O			00
00-051-0656	S	Li3 C8	Lithium Graphite	H			40
00-055-1157	S	C60 ·2 C H Br3	Fullerene bromoform	H	4.572010	4.419550	6.692790
01-088-1596	S	Sn Ta S2	Tin Tantalum Sulfide	H	4.358100	2.719570	2.039080

Sorted by SYS (Crystal System)

Special Order Sort

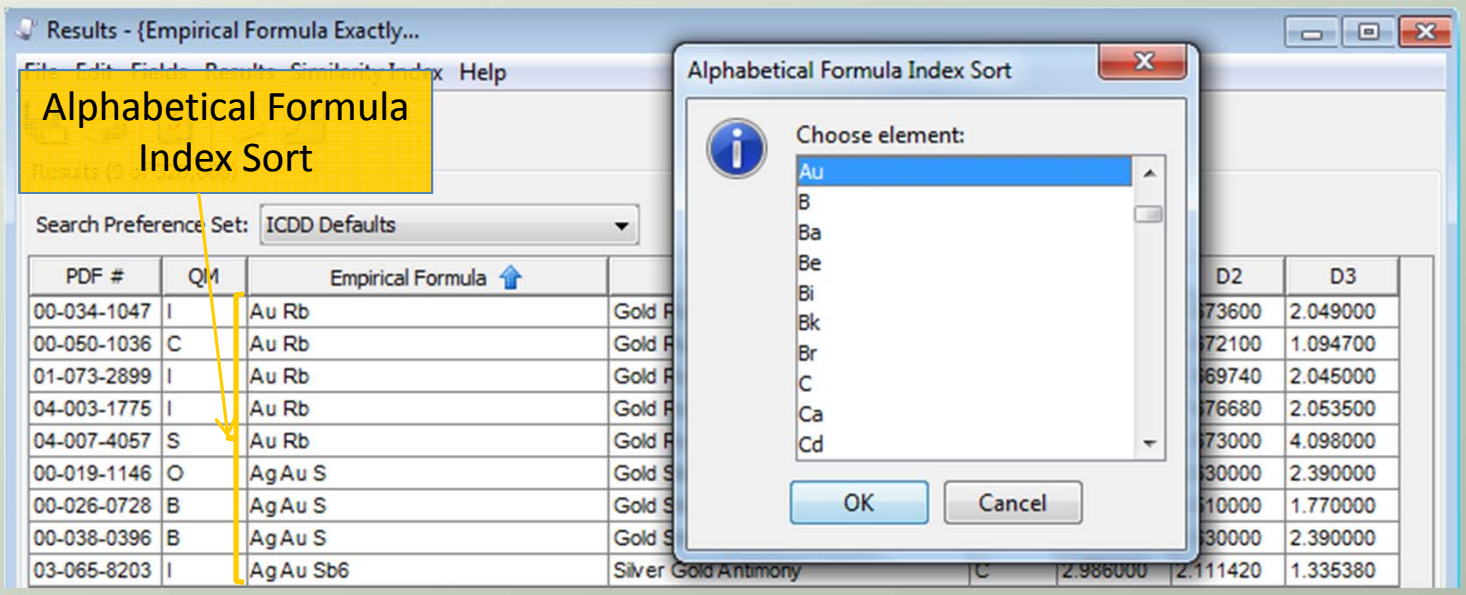
- This can be performed by:
  - Left-clicking a *Special Order* sort column.
  - Or right-clicking a *Special Order* sort column and selecting *Sort by Special Order*.
- Sorting on a column twice will perform a descending sort.



Sorted by Pearson Symbol Code

Alphabetical Formula Index Sort

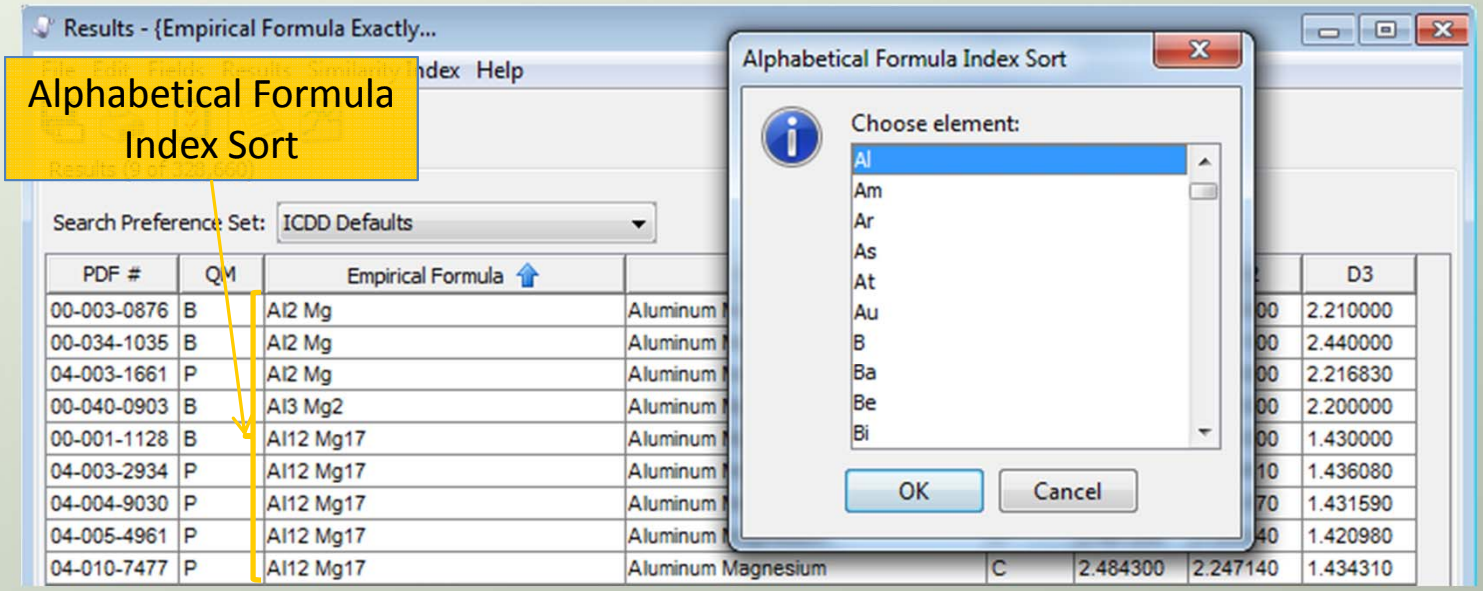
- The *Alphabetical Formula Index Sort* will sort the Empirical Formula column based on a specific sort element.
- Formulae are sorted by elements alphabetically starting with the sort element.
- Example 1: **Al**, **Al** S, **Al** Si - sorted on **Al**
  - This example shows a basic alphabetical sort.
- Example 2: **Au** Rb, Ag **Au** S, Ag **Au** Sb_6 - sorted on **Au**
  - Since sorting starts with the sorting element first, "Ag Au Sb_6" comes last because Rb comes before S and Sb.



Example 2

Alphabetical Formula Index Sort

- If 2 formulae elements are alphabetically equal and contain 2 or 3 elements, they are sorted by the ratio of the second-to-last divided by the last atomic weight from largest to smallest.
- Example 3: **Al**$_2$ Mg, **Al**$_3$ Mg$_2$, **Al**$_{12}$ Mg$_{17}$ - sorted on **Al**
  - Since these are all alphabetically equivalent and are a binary system, they are sorted on their last 2 elements. The ratios are 2/1, 3/2, and 12/17. **Al**$_2$ Mg is first because 2 is the larger than 3/2 and 12/17.
- Example 4: **Al**$_2$ Mg$_5$ Se$_8$, **Al**$_2$ Mg$_2$ Se$_5$ - sorted on **Al**
  - Since these are all alphabetically equivalent and are a ternary system, they are sorted on their last 2 elements. The ratios are 5/8, and 2/5. **Al**$_2$ Mg$_5$ Se$_8$ is first because 5/8 is the larger than 2/5.



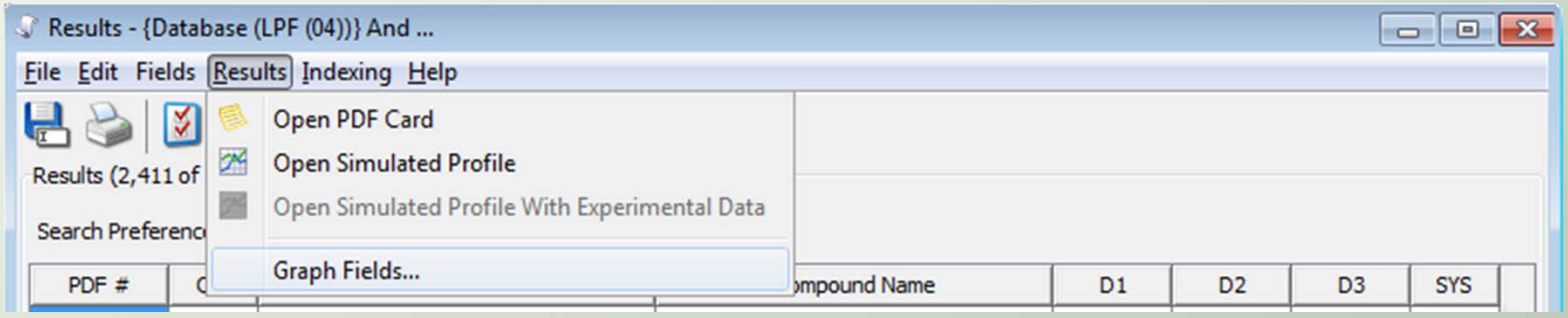
Example 3

Alphabetical Formula Index Sort

- If formulae elements are alphabetically equivalent and higher than a ternary system, atomic weights are sorted alphabetically.
- Example 5: Nb **S** Se_2 Sn, Nb **S** Se_2 $Sn_{0.50}$ - sorted on **S**
  - Since these are all alphabetically equivalent and are higher than a ternary system, they are sorted by their atomic weights alphabetically starting with the sort element. The first difference in atomic weight is Sn. Even though there is 1 Sn implied, it is not written and Nb S Se_2 Sn is listed first.

Graphing

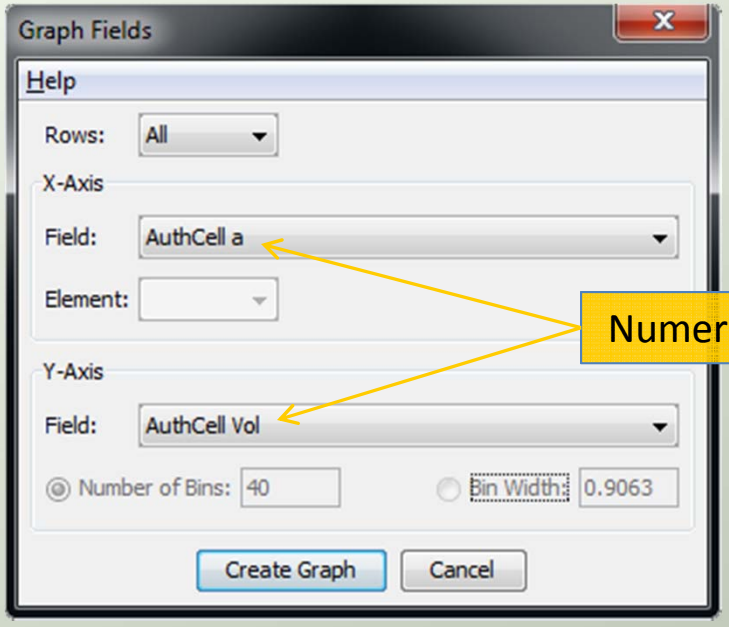
- The Results table can be graphed using any display field.
- To graph a field, click the Results menu and select *Graph Fields*.



- Depending on the display field(s) selected, there are three different types of graphs available:
  - X-Y graph
  - Histogram
  - Category graph

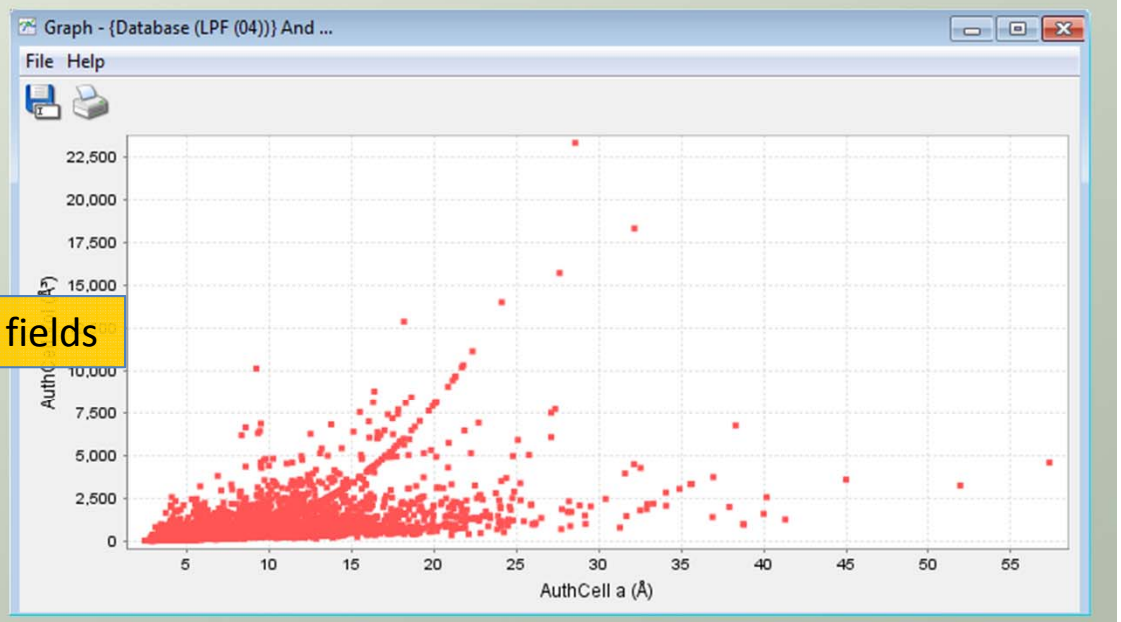
Graphing - X-Y Graph

- If the x-axis field and y-axis field are both numeric fields, then an X-Y graph will be displayed.
- You can limit the rows to be graphed by pre-selecting the rows in the Results table first. Otherwise, the graph will use all rows as indicated by the *Rows* selection box.



Graph Fields form

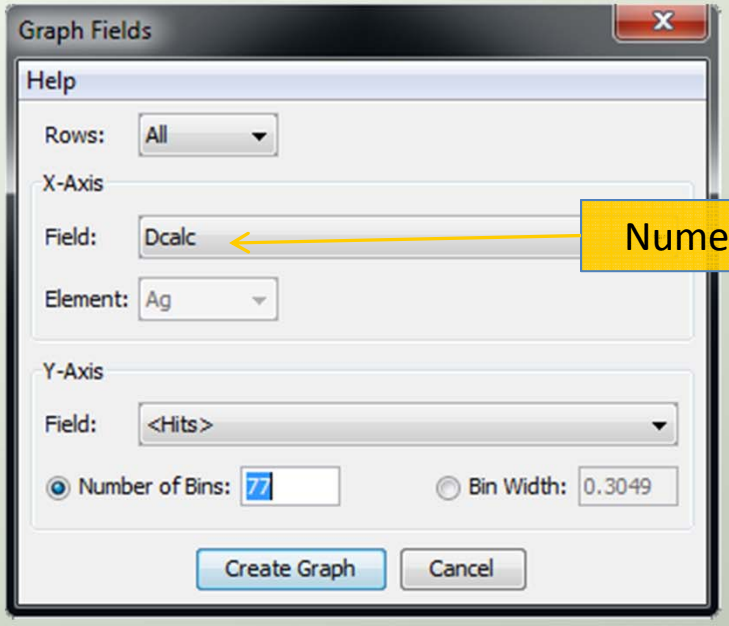
Numeric fields



X-Y graph of author's cell volume and author's cell a

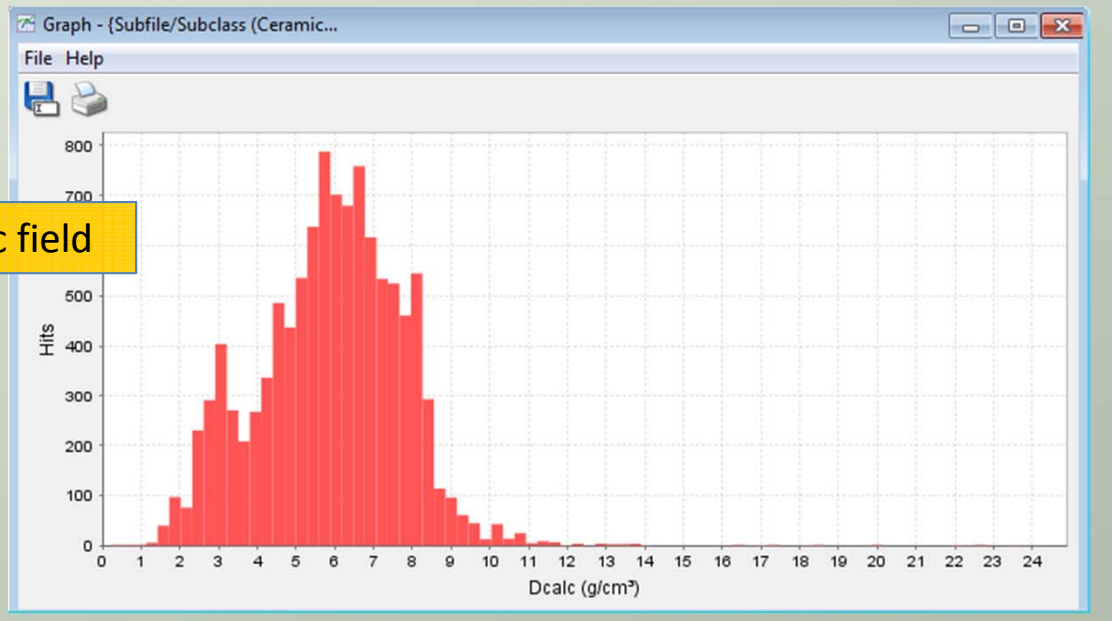
Graphing - Histogram

- If the x-axis field is a numeric field and the y-axis field is <Hits>, then a histogram will be displayed.
- Individual element values for the weight % and atomic % x-axis fields can be selected in the *Element* listbox.
- You can customize the histogram bin (bar) distribution by changing the *Number of Bins* or *Bin Width* values.



Numeric field

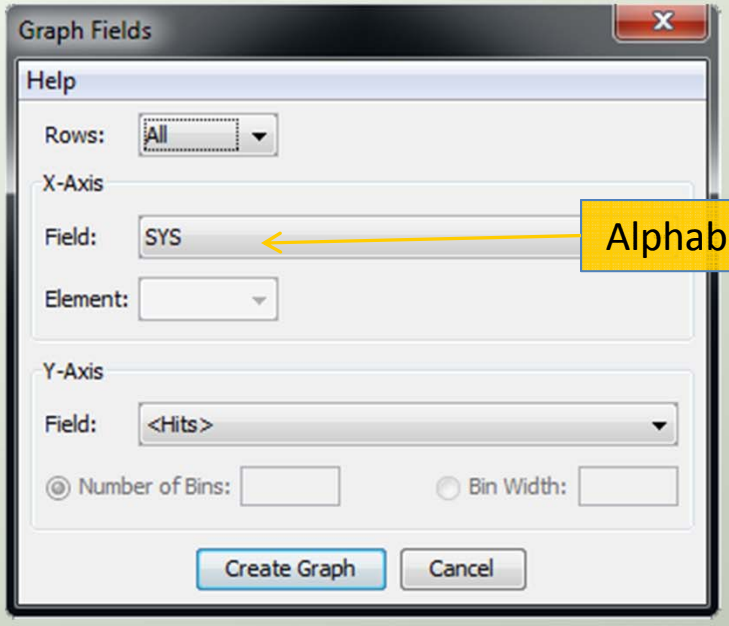
Graph Fields form



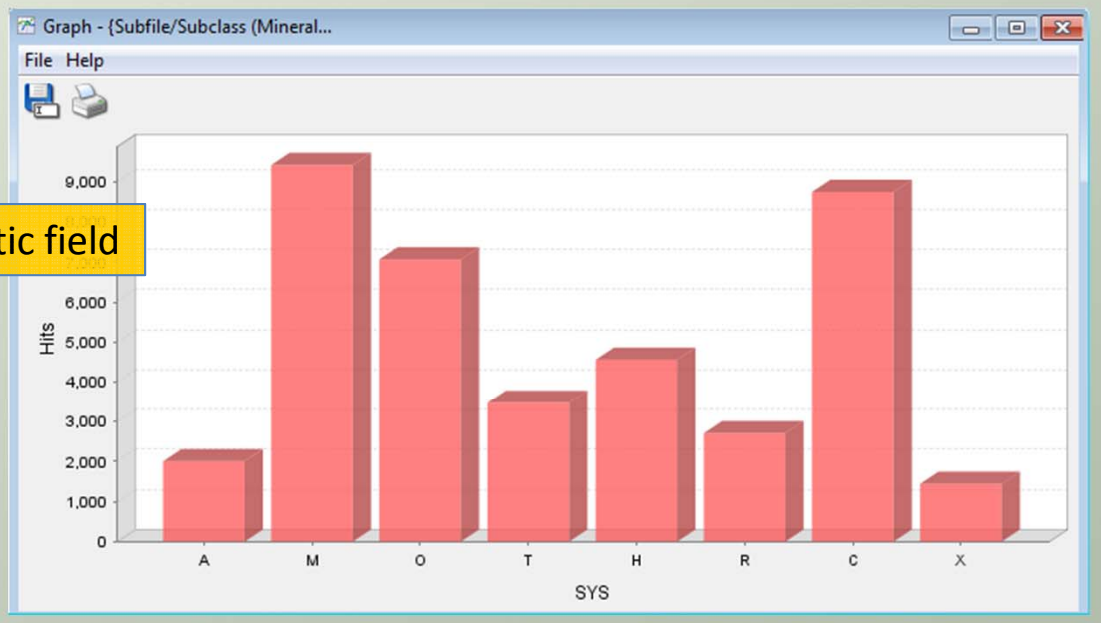
Histogram of the calculated densities for all ceramics

Graphing – Category Graph

- If the x-axis field is an alphabetic field, then a category graph will be displayed.
- The y-axis field will default to <Hits>, indicating that the y-axis represents the number of entries for each unique x-axis value (category).



Graph Fields form



Category graph of the crystal system distribution for all minerals

Thank you for viewing our tutorial.
Additional tutorials are available at the ICDD website.
www.icdd.com

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