

Using Subfiles with PDF-4/Organics

Using Subfiles – What ?

- PDF-4/Organics has some uniquely defined and populated subfiles these include

– Excipients	1,623 Entries*
– Bioactivity	9,010
– Pharmacueticals	3,577
– Merck	1,574

These subfiles are expressly designed to solve pharmaceutical material identifications.

* PDF-4 / Organics Release 2008

Unique Subfiles

Expert knowledge put in the database !

- **Excipients** – Defined by USP and European standards , edited by ICDD editors
- **Bioactivity** – Defined and edited by CSD* editors using author cited criteria, can be commercial or exploratory materials
- **Pharmaceuticals** – Defined and edited by ICDD editors as being commercial materials
- **Merck** – Materials having corresponding entries in the Merck Handbook as defined by an ICDD member task group

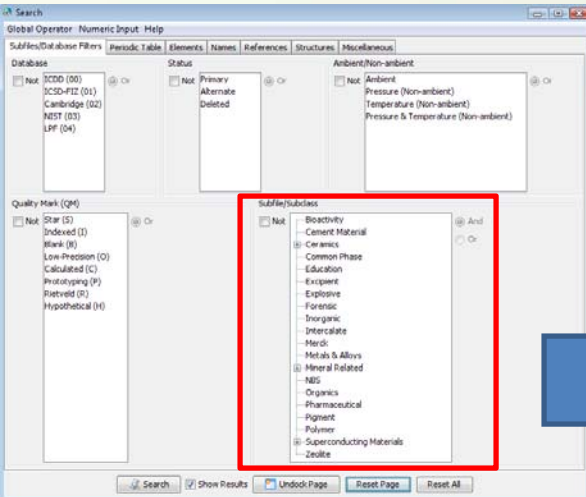
Using Subfiles – Why ?

- Faster Searches – only use chemistry of interest
- Increased efficiency – fewer false positive matches

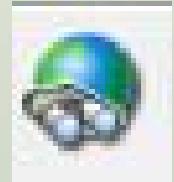
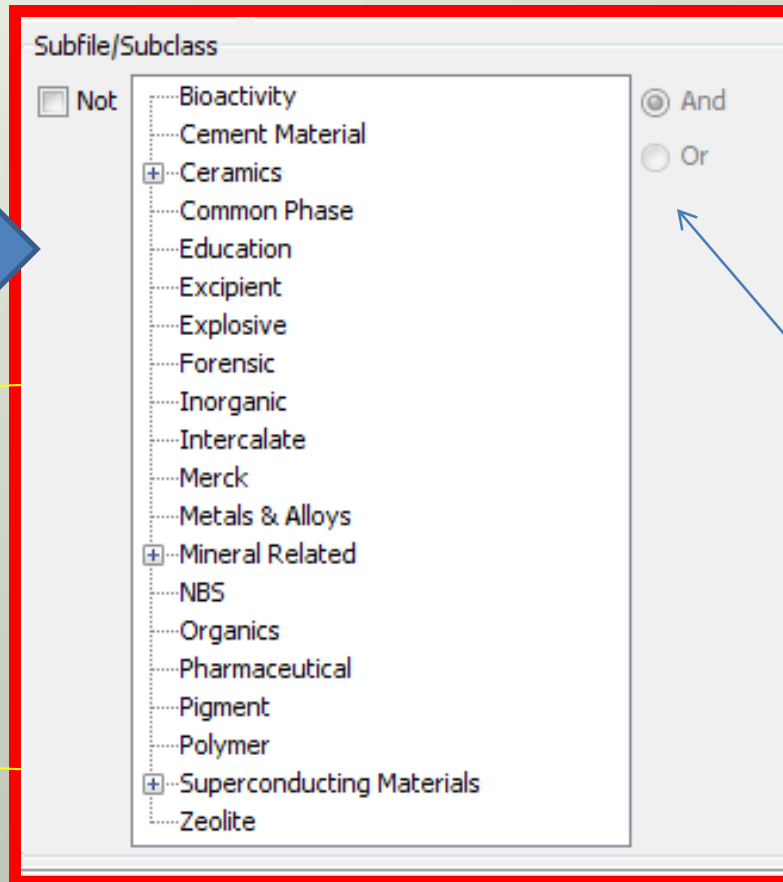
Using Subfiles – How?

- The easiest way to use a subfile is to point and click a defined subfile of interest (i.e. pharmaceuticals, excipients etc).
- User defined subfiles can also be created and saved through keyword and other various searches

Selecting a Subfile from the Search Page



“Point and Click”
Selection

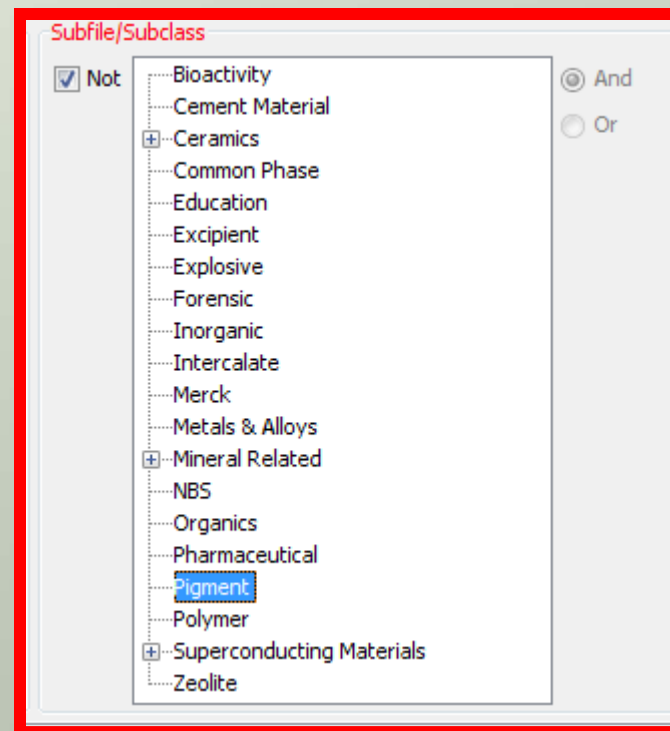
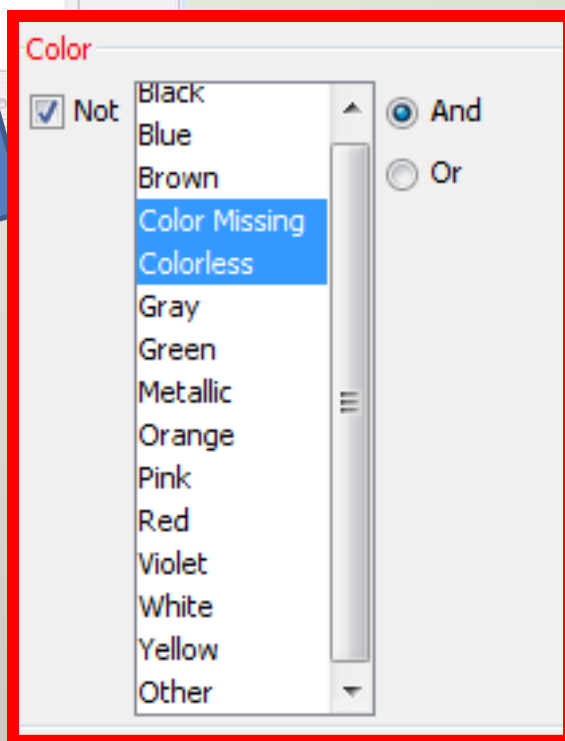
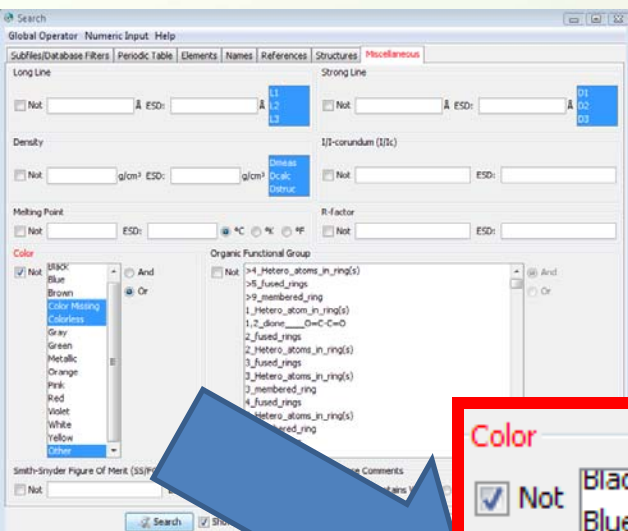


Search
Icon

Boolean
Operators

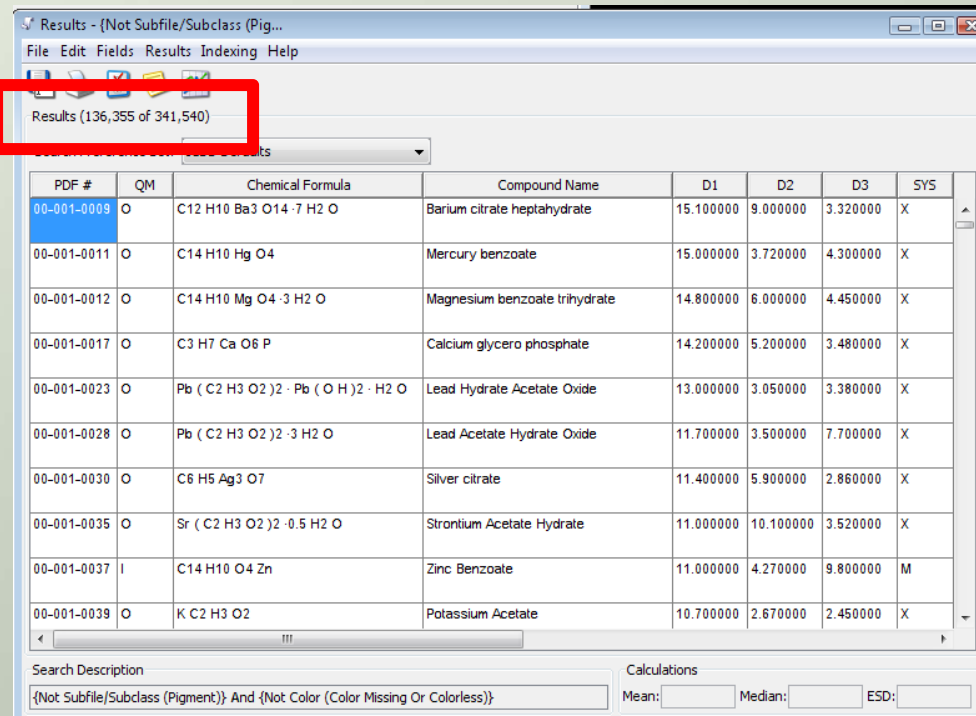
Example of a user defined subfile

If a scientist wanted to create a subfile of pigment candidates. The following search would eliminate colorless compounds and color missing compounds from the database. These results could then be combined to subtract the known commercial pigments using the “not” operator on the pigment subfile.



User defined subfile

The user defined subfile of colored materials that aren't known pigments found 136,355 materials from 341,540 possible entries



Results (136,355 of 341,540)

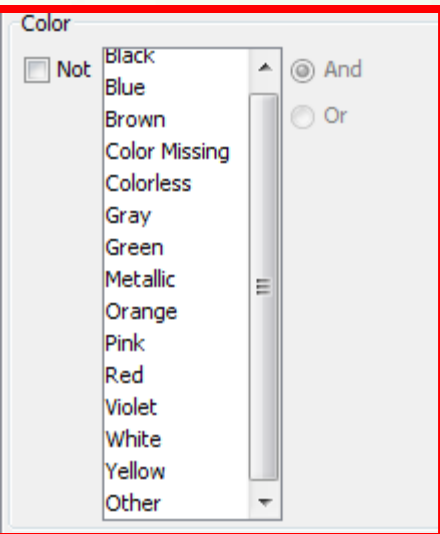
PDF #	QM	Chemical Formula	Compound Name	D1	D2	D3	SYS
00-001-0009	O	C ₁₂ H ₁₀ Ba ₃ O ₁₄ · 7 H ₂ O	Barium citrate heptahydrate	15.100000	9.000000	3.320000	X
00-001-0011	O	C ₁₄ H ₁₀ Hg O ₄	Mercury benzoate	15.000000	3.720000	4.300000	X
00-001-0012	O	C ₁₄ H ₁₀ Mg O ₄ · 3 H ₂ O	Magnesium benzoate trihydrate	14.800000	6.000000	4.450000	X
00-001-0017	O	C ₃ H ₇ Ca O ₆ P	Calcium glycerol phosphate	14.200000	5.200000	3.480000	X
00-001-0023	O	Pb (C ₂ H ₃ O ₂) ₂ · Pb (O H) ₂ · H ₂ O	Lead Hydrate Acetate Oxide	13.000000	3.050000	3.380000	X
00-001-0028	O	Pb (C ₂ H ₃ O ₂) ₂ · 3 H ₂ O	Lead Acetate Hydrate Oxide	11.700000	3.500000	7.700000	X
00-001-0030	O	C ₆ H ₅ Ag ₃ O ₇	Silver citrate	11.400000	5.900000	2.860000	X
00-001-0035	O	Sr (C ₂ H ₃ O ₂) ₂ · 0.5 H ₂ O	Strontium Acetate Hydrate	11.000000	10.100000	3.520000	X
00-001-0037	I	C ₁₄ H ₁₀ O ₄ Zn	Zinc Benzoate	11.000000	4.270000	9.800000	M
00-001-0039	O	K C ₂ H ₃ O ₂	Potassium Acetate	10.700000	2.670000	2.450000	X

Search Description: {Not Subfile/Subclass (Pigment)} And {Not Color (Color Missing Or Colorless)}

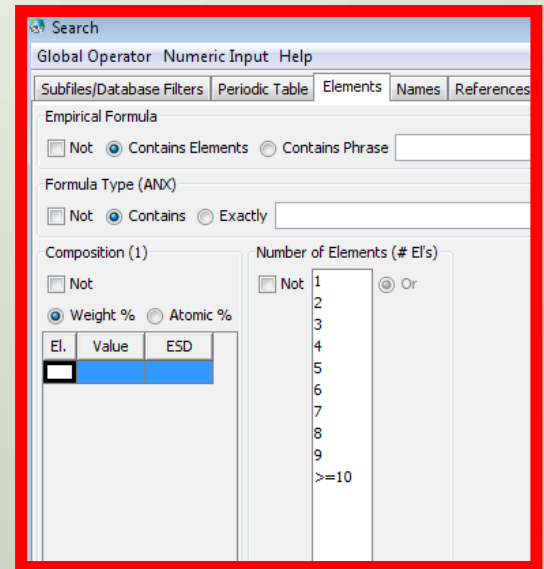
Calculations: Mean: Median: ESD:

User Defined Subfiles

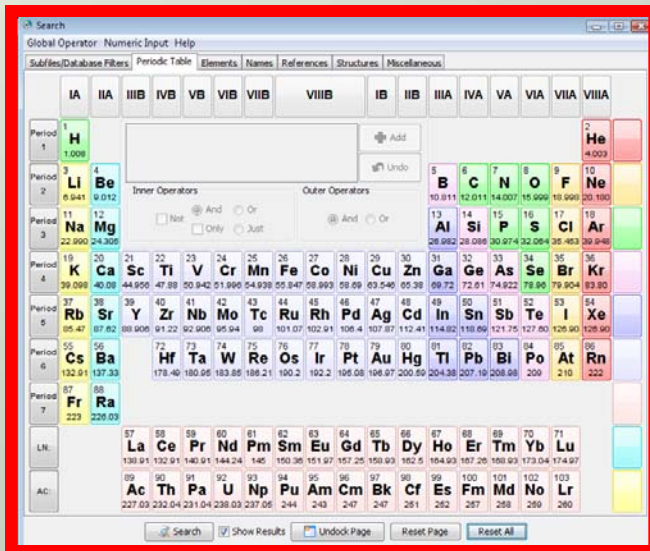
further refinements of a pigment candidate search



The user could further narrow the search by choosing specific colors of interest



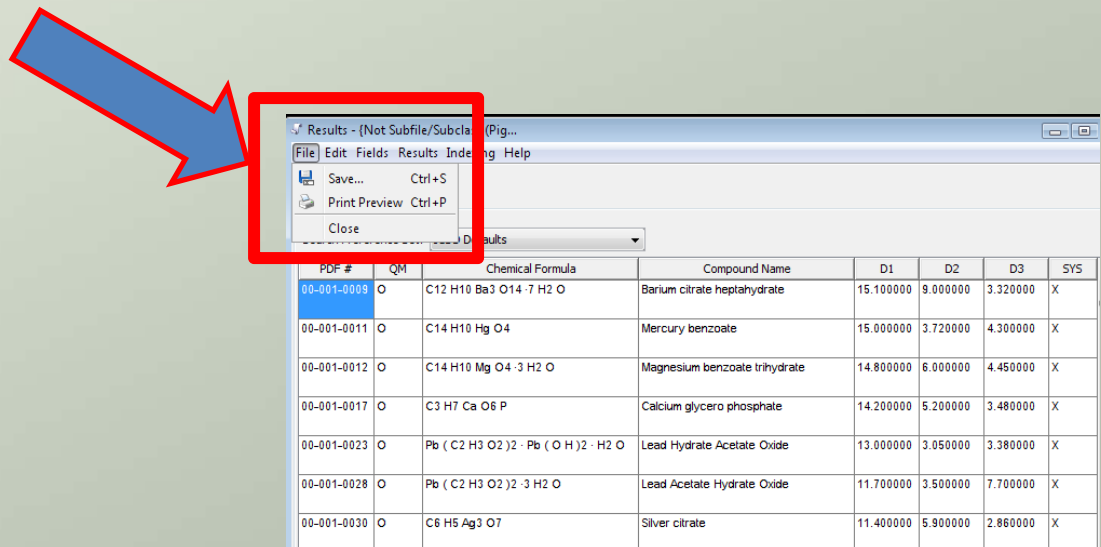
The "Element" Search page could reduce the search to specific compositions



The periodic table search could be used to eliminate known heavy metals and radioactives

User Defined Subfiles

- Searches can be combined by using the History function
- Searches can be saved from the Results form



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00-001-0012	O	C ₁₄ H ₁₀ MgO ₄ ·3H ₂ O	Magnesium benzoate trihydrate	14.800000	6.000000	4.450000	X
00-001-0017	O	C ₃ H ₇ CaO ₆ P	Calcium glycerol phosphate	14.200000	5.200000	3.480000	X
00-001-0023	O	Pb(C ₂ H ₃ O ₂) ₂ ·Pb(OH) ₂ ·H ₂ O	Lead Hydrate Acetate Oxide	13.000000	3.050000	3.380000	X
00-001-0028	O	Pb(C ₂ H ₃ O ₂) ₂ ·3H ₂ O	Lead Acetate Hydrate Oxide	11.700000	3.500000	7.700000	X
00-001-0030	O	C ₆ H ₅ Ag ₃ O ₇	Silver citrate	11.400000	5.900000	2.860000	X