Finding Coordination Compounds in SciFinder – a Quick Guide

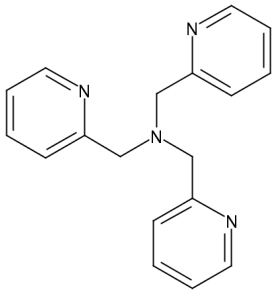
If you don't already have a personal SciFinder account, you must first register for one here: http://www.lib.utexas.edu/chem/scifinder.html (You'll have to use your utexas.edu email address.) Log in to SciFinder on-campus here: https://scifinder.cas.org/ (if you're off campus, use the proxied link from the Chemistry Library home page.)

Searching for organometallic and coordination compounds in SciFinder can be tricky. If you want to find a *specific* complex, starting with a **molecular formula** is often easier, as long as you count the atoms correctly. (See the related handout on doing this.) Alternately, you can draw the **exact structure** using the structure editor, though it's easier to find and modify a similar structure than to draw it from scratch. Searching by chemical name is the least advisable method: the nomenclature rules for organometallic compounds are far too complex and varied to allow reliable searching for a specific complex.

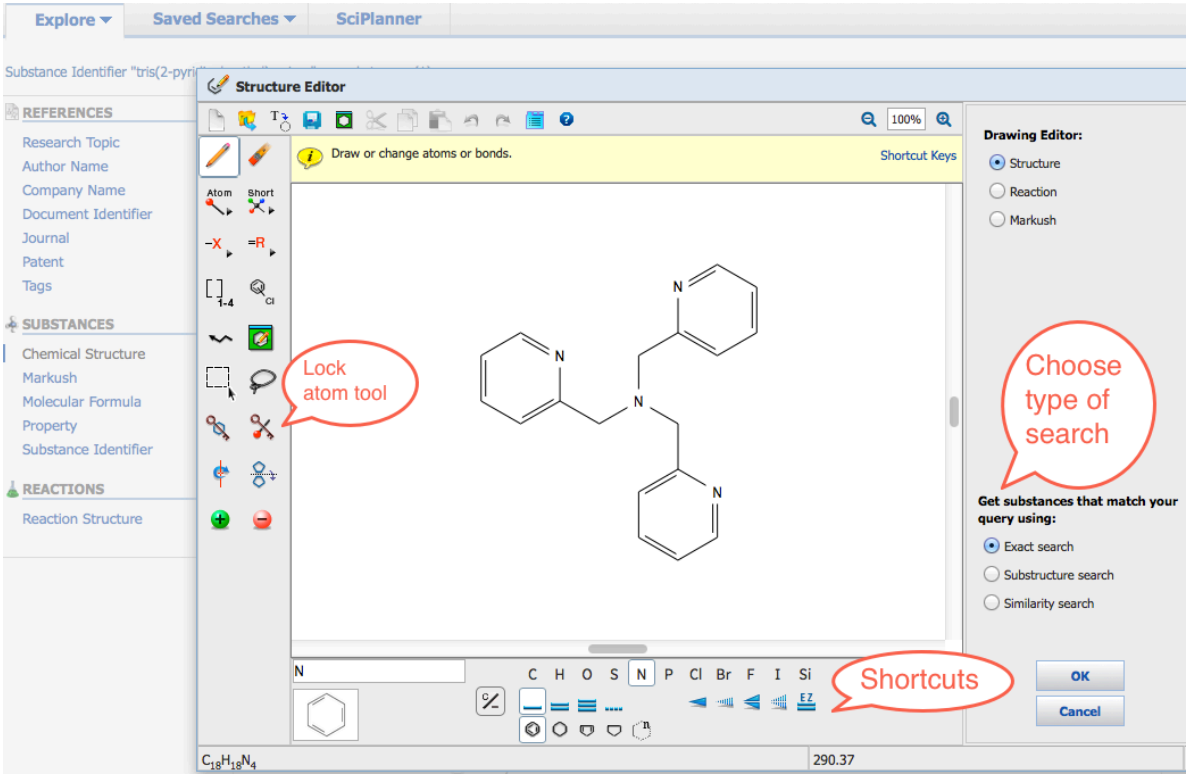
Even more straightforward is to start with the organic ligand, and work from there.

First, let's look at a simple search for a ligand, and in part II we'll look at a way to find it in coordination compounds.

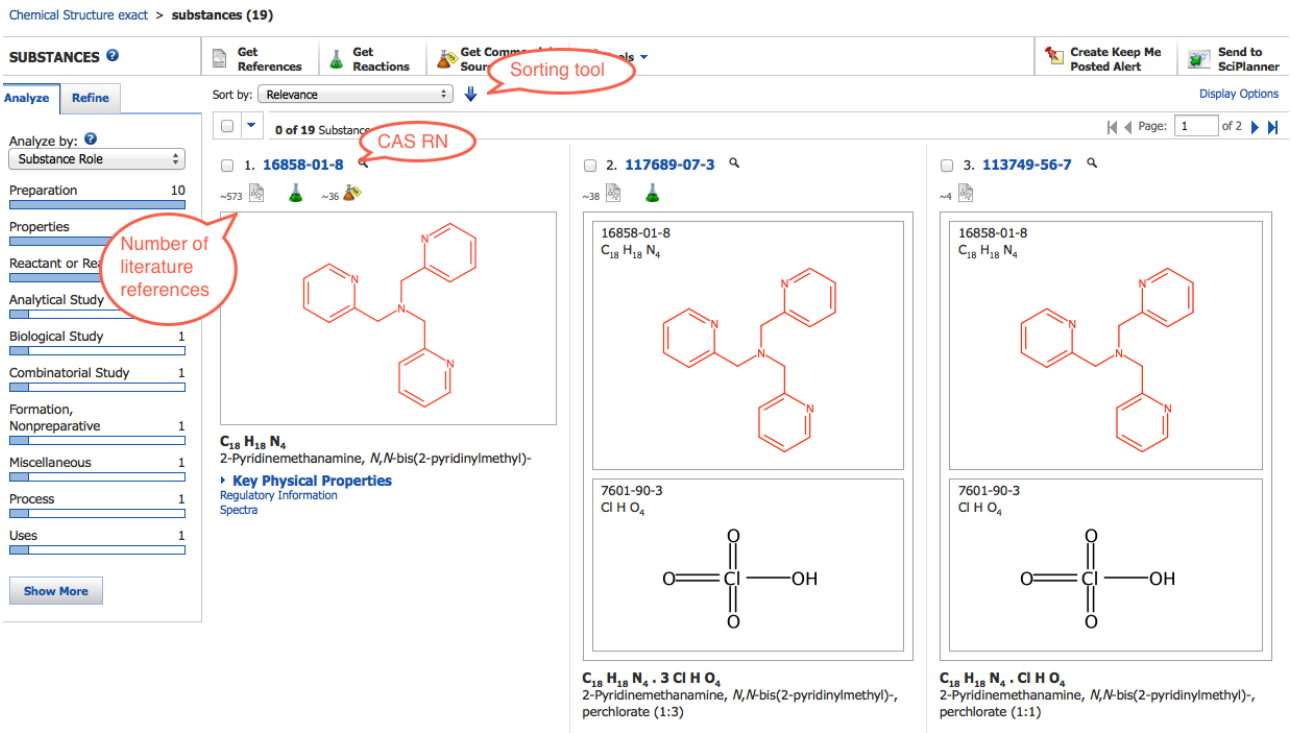
I: Find literature about the synthesis of this molecule:



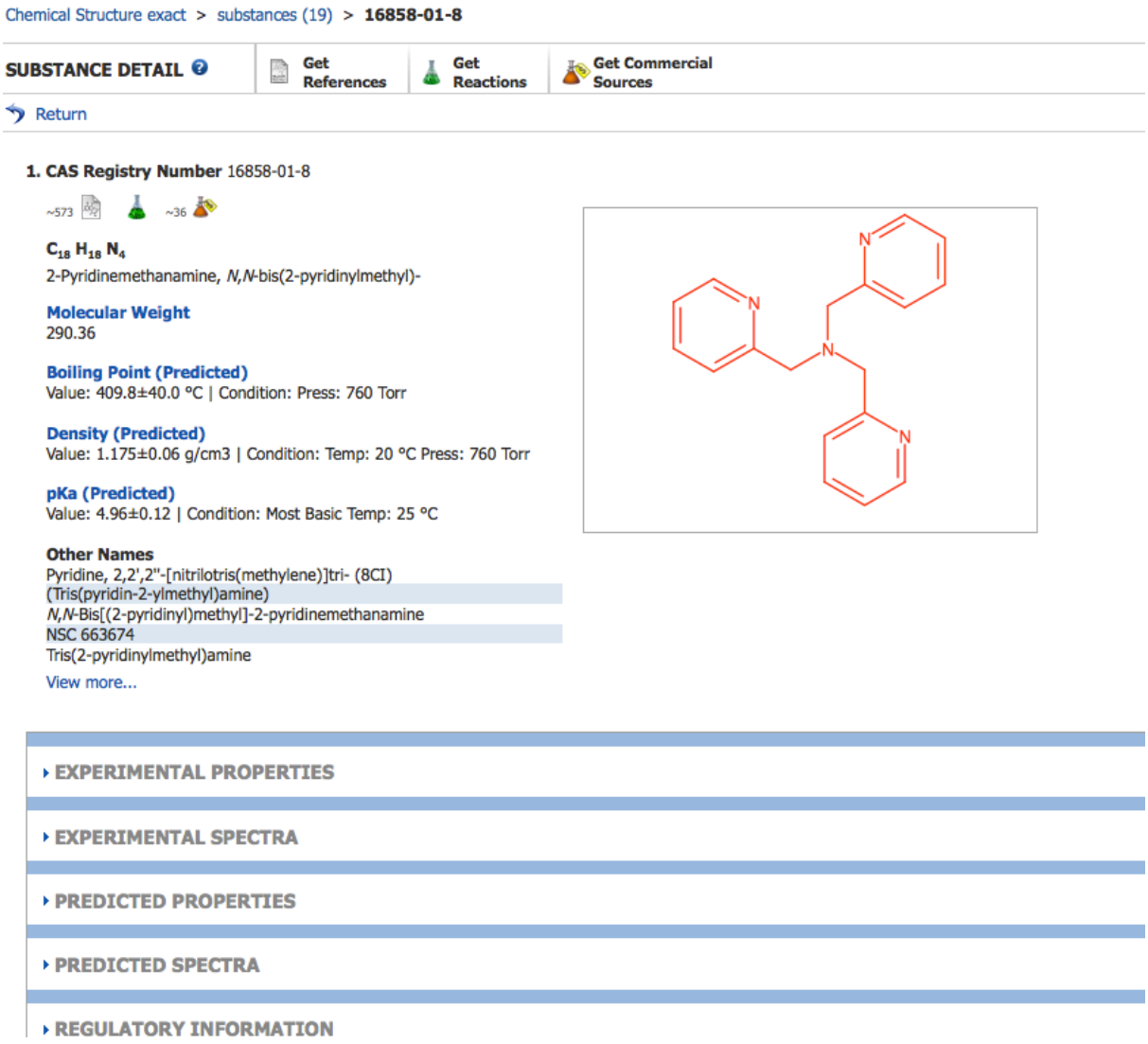
Log into SciFinder, and choose Explore Substances – Chemical Structure. Open the structure editor and draw this structure using the tools provided. Note there are shortcuts to drawing rings. You can change atoms after you draw the skeleton. It doesn't have to be pretty! Select **Exact Search** if you're looking for this structure only, with no substitutions or other parts. When you're done, click OK in the editor window, then Search.



The exact search will retrieve all records where this structure is a standalone component. Your target structure is highlighted in red. The compounds are sorted by "relevance" but you can re-sort the results if you wish. Generally you should be looking for the ones that have the most literature references, implying that they are the best-described in the literature.

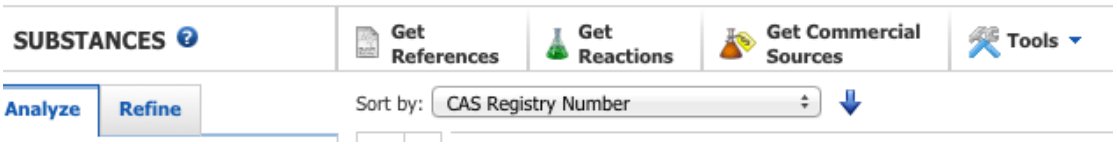


Click on the structure or Registry Number to open the full record for the compound you want.



The full display shows the **CAS Registry Number (RN)**, a unique identifier in the CAS databases. You can use RNs later for other searches as a shortcut to drawing structures or pulling up these records again. The RN for this compound is **16858-01-8**. Here you can also see the official CA Index Name for this substance, and other synonyms that have been used in the literature. (Note the complexity and diversity of names.) Many substance records include various experimental physical and spectral data fields, with corresponding source literature references, but these are selective, not comprehensive.

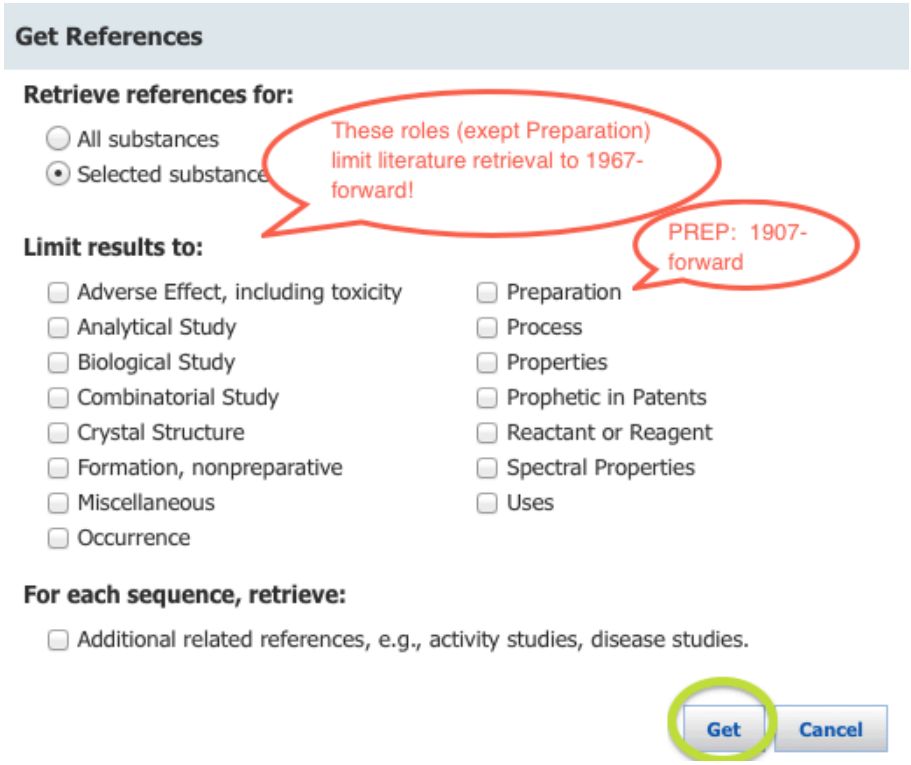
The toolbar offers a number of options for your next step:



- **Get References** pulls up bibliographic records (since 1907) that have mentioned this substance.
- **Get Reactions** pulls up a list of reactions (mostly since 1985) that involve this substance. You can refine and sort the reactions by many parameters, including the substance's role (product, reactant, catalyst, etc.), yield, number of steps, year, and so on.
- **Get Commercial Sources** retrieves a table of suppliers who sell this chemical.

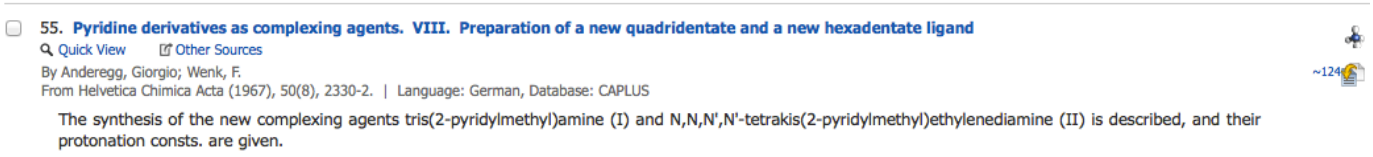
When you select Get References, you see a selection box for **CAS Roles**. These are descriptors that indicate the primary *context* of the substance's presence in a document. If you're looking for anything other than prep methods, it's generally best to avoid selecting roles here, for two reasons: 1) they limit your retrieval to post-1967 publications, and 2) they may cause you to miss useful references because something you're interested in may not have been designated by Chemical Abstracts' indexers as a primary focus of the document. (This is often the case when looking for characteristic physical and spectral properties of a synthesized compound.) The exception is the **Preparation** role, which has been extended back to 1907.

Since we're interested in papers on the synthesis of this molecule, choose Preparation and click Get.



The next screen shows literature references in reverse-chronological order (newest on top). Now you can use the Refine, Analyze, and Categorize tools to narrow your results and zero in on what you're most interested in. Then you can scan the abstracts for references that look promising.

> TIP: Articles reporting the synthesis of a molecule are often the *earliest* ones in a result set (obviously). Scroll to the bottom or re-sort the list to find them. In this case, the earliest reference is a 1967 paper in the journal *Helvetica Chimica Acta* describing the synthesis of a "new" ligand.



Clicking on the title pulls up the full record for the article. Here you can see the context (role) of the substance in the article, as determined by CAS indexers, along with a list of other Registry Numbers mentioned in the document, and more general subject vocabulary terms.

If you want to look at the actual article, click the **Other Sources** button. This button appears on every record, but it doesn't necessarily mean that a digital version exists, or that if it does exist, you'll actually have access to it. For journal articles, the button starts a search in UT-Austin's local system to see if we have full text access or not. (This linking is not perfect, and sometimes misses the target.) In some cases we don't have electronic access, but we may have the journal in – GASP! – print, which is more likely for older publications. If UT doesn't have it at all, you can request a copy from Interlibrary Services. In this example, we don't have electronic access to the article, but the Library Catalog indicates that the print journal is located in the Chemistry Library. (Don't be afraid to come in and use a printed journal! You can scan the article for free using one of our scanners.)

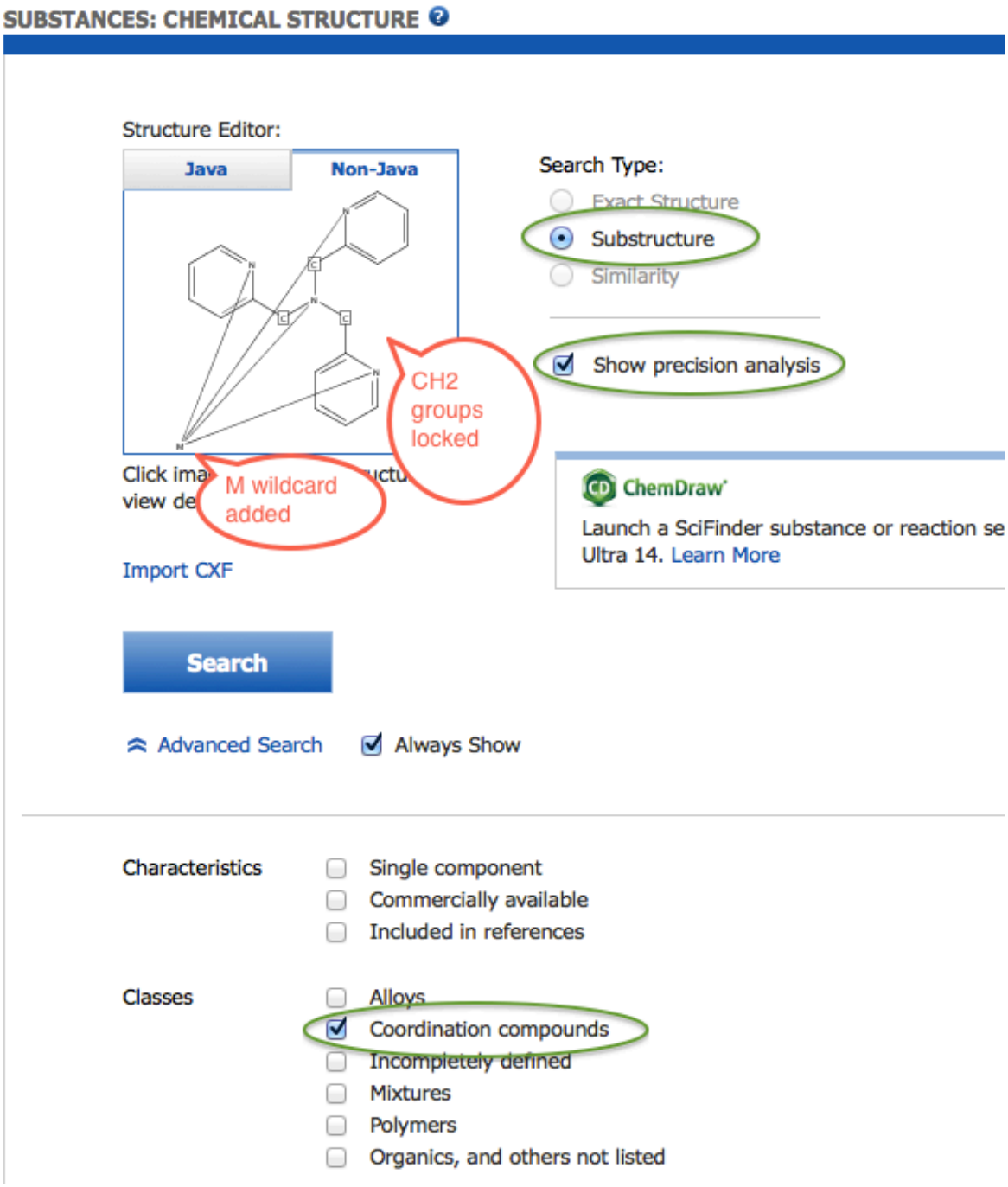
Sometimes it's useful to see what later papers have **cited** a particular article, as a follow up method to your search. SciFinder makes this easy: just click the little paper button on the right of the brief display, or click the Get Related Citations (Get Citing) button in the full display. This pulls up all the references (since about 1995) that have cited the article in question.

II. Find Coordination Complexes with this Ligand

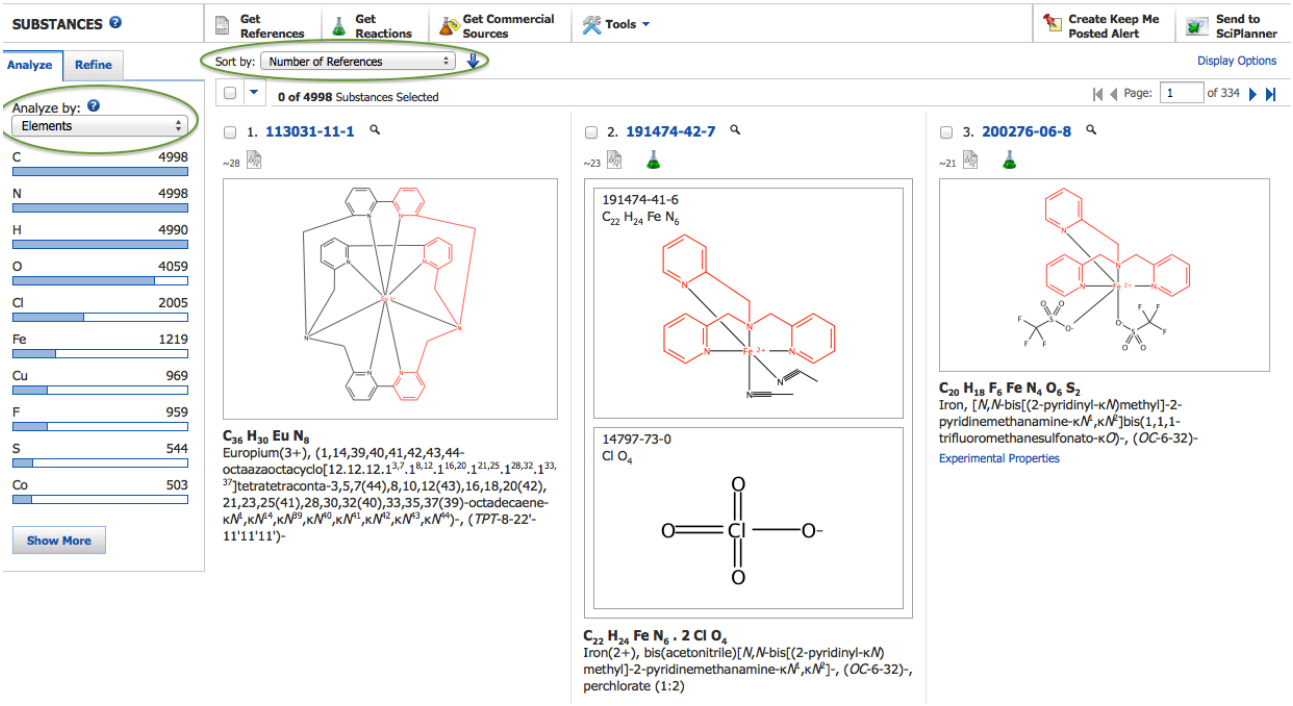
There are several ways you could approach this, but the easiest is to start from your original structure search, or launch a new one by mousing over the structure diagram for the ligand, clicking the little **>>** arrow in the top right corner to see More Options, and choosing Explore by Structure/Chemical Structure in the pop-up menu. SciFinder will then import that structure into the drawing tool and you can modify it as you wish.

If you know how the metal is bonded in the complex, you can add an element symbol or an "M" node (a wildcard for any metal) to the structure and draw bonds from it to all of the appropriate atoms in the ligand. (In this example, all four nitrogens.) You can also use the Lock tools to block substitution at selected atoms or rings. In this example we've locked the three CH_2 groups in the ligand to prevent further substitution at those nodes. This will limit and focus your results.

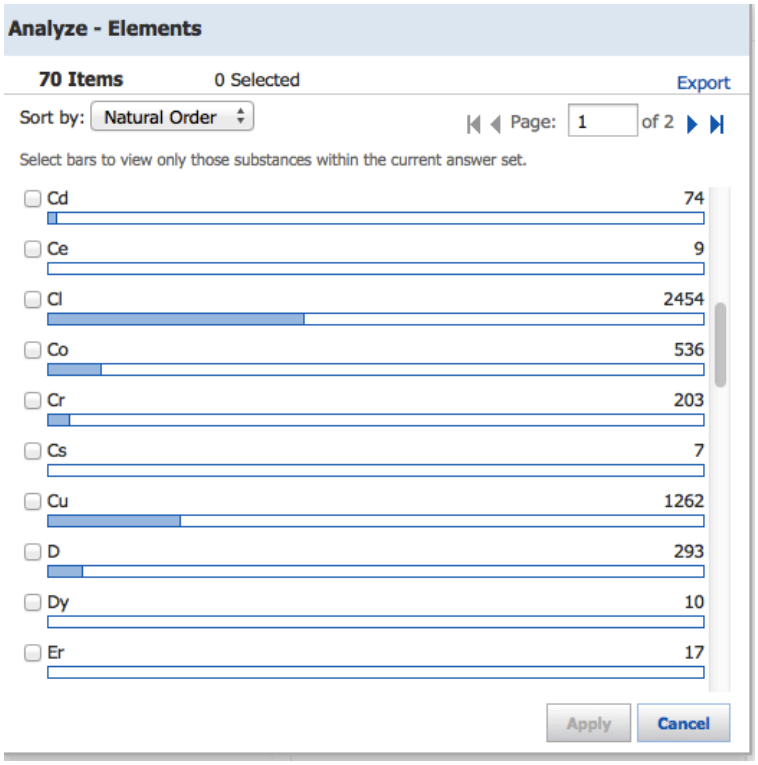
When you transfer the structure to the search screen, SciFinder will warn you about overlapping bonds and nonstandard valencies. Just click through to continue; these are expected in coordination compounds. On the search screen, change the search type to "Substructure" and select "Show Precision Analysis," and choose the limiter for Coordination Compounds.



Click Search. From the Precision Analysis histogram, choose the "Conventional Substructure" results. The number of substances may be very large, but most of the records will have only one or even zero literature references, and even the most-reported complexes may only have a few dozen references. Sort the results by Number of References to bring the best-characterized complexes to the top.



Note how the coordination structures are drawn in the database, and how they are named. To see what metals are represented, you can use the **Analyze** tool on the left, select **Elements**, then Show More, and look through the table by either Frequency or Natural Order. You can then select some target elements and click Apply, and it will limit your results set accordingly.



Alternatively, try using the **Refine** tool and limit the set by Atom Attachments to filter by specific elements bonded to an atom you select.

From the Substances results list, you can choose one or more compounds and retrieve the literature references for them as described in part I above.

You can save substance and reference answers in your SciFinder account, or mark and export them to external files. Any unsaved work will be deleted when you log out.

More SciFinder training materials, videos, and tutorials can be found at http://www.cas.org/training/scifinder. Our own FAQ guide can be found at http://www.lib.utexas.edu/chem/scifinder_faq.html.

If you need help or a live demonstration of these techniques, contact the Chemistry Librarian and set up an appointment.

NOTE: A thorough search for substances in SciFinder should be followed up with a similar search in **Reaxys**, an important complementary tool for organic and inorganic chemistry. See http://www.lib.utexas.edu/info/reaxys.html for more information.

For additional help on how to use SciFinder:
1) Refer to this suite of YouTube videos ("SciFinder Need-To-Know" playlist):
https://youtu.be/2s-KpZ5tYBs?list=PLB5yoyDBtQbWofS6c7g1riYrc2nD1Y3BR
2) Ask your TA