Reaxys Training

How to Find Organometallic and Coordination Compounds in Reaxys

April 2012

reaxys.com

Reaxys application version: 2.11926

MarvinSketch version 5.8.2

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Practice Exercises

Introduction

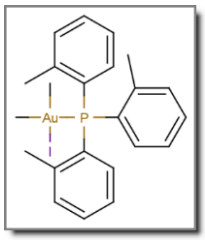
The data, structures, and reactions for organometallic and coordination compounds in Reaxys come from the literature and patents.

Information from the literature - information covering the literature from 1817-1975 was originally obtained from the *Gmelin Handbook of Inorganic and Organometallic Chemistry*, (including all main volumes and supplements). Information from 1976 to the present has been extracted from selected inorganic, organometallic, physical chemistry, and solid state journals.

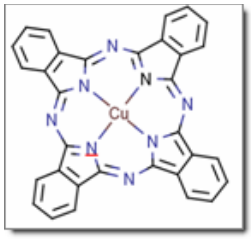
Information from patents - The historical **patent information** covers patents from the early 1800's to about 1980. The information abstracted from those patents includes substance and reaction data, and patent citation information (patent assignee, authors, patent number, patent year, and country code).

The **in-depth** patent information covers patents from about 1976 to the present. These patents are English language patents from World, US, and European patent offices. In addition to the type of information mentioned in the previous paragraph, also included are all patent family members (all patent numbers and application numbers for an indexed patent), Markush substance display, prophetic substances*, and patent classification codes.

The Substances



Organometallic Compound



Coordination Compound

Organometallic compounds contain at least 1 carbon bonded to at least 1metal/metaloid.

Coordination compounds contain at least one metal bonded to another atom by a coordinate covalent bond.

Organometallic compounds and coordination compounds with known manner of ligand coordination are stored with the complete formula and structure, e.g., Fe(C5H5)2

Organometallic salts and ionic coordination compounds with known manner of ligand coordination are divided into cations and anions. The complete structures of the ions are available, e.g., [Co(NH3)6](3+)*3Cl(1-)=[Co(NH3)6]Cl3.

Organometallic compounds and coordination compounds with unknown manner of ligand coordination are divided into fragments by separating all ligands from the metal center, e.g., If there is an unknown coordination of thiocyanate to Co(3+) in [Co(NH3)5(SCN)]Cl2 (coordination by N or S atom possible), theformula is given as Co(3+)*5NH3*SCN(1-)*2Cl(1-)=[Co(NH3)5(SCN)]Cl2. The separated fragments are available with their structures

Searching Tips

The preferred way to search for **specific organometallic and coordination compounds** is by structure. You can either use the Reaxys functionality to generate the structure by name or you can use a structure editor to draw the substance.

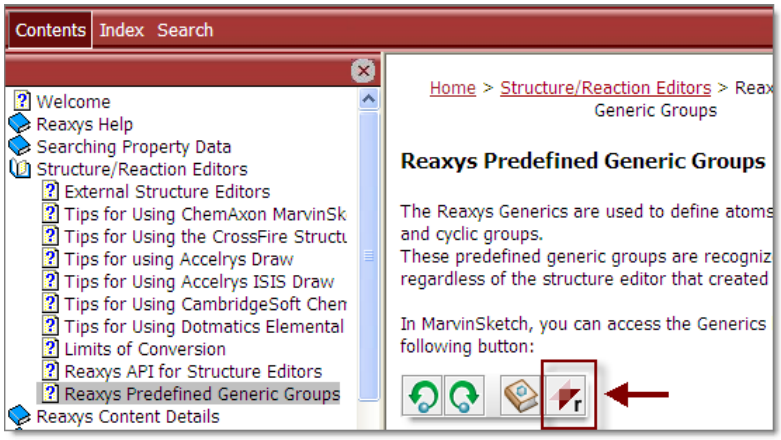
Searching by **name** and searching by **formula** will most likely yield relevant results, but you may also be missing results that would have been obtained with a structure search.

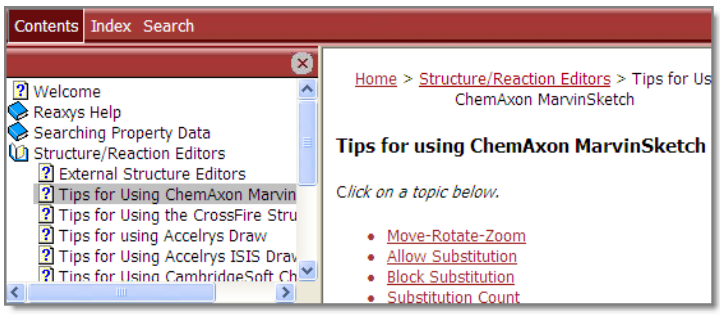
Searching by **name** is less preferred than by structure because not all compounds have complete names. The names found in Reaxys are extracted exactly as the authors of the original documents spelled them. In some cases names may be ambiguous, non-systematic or simply not available at all.

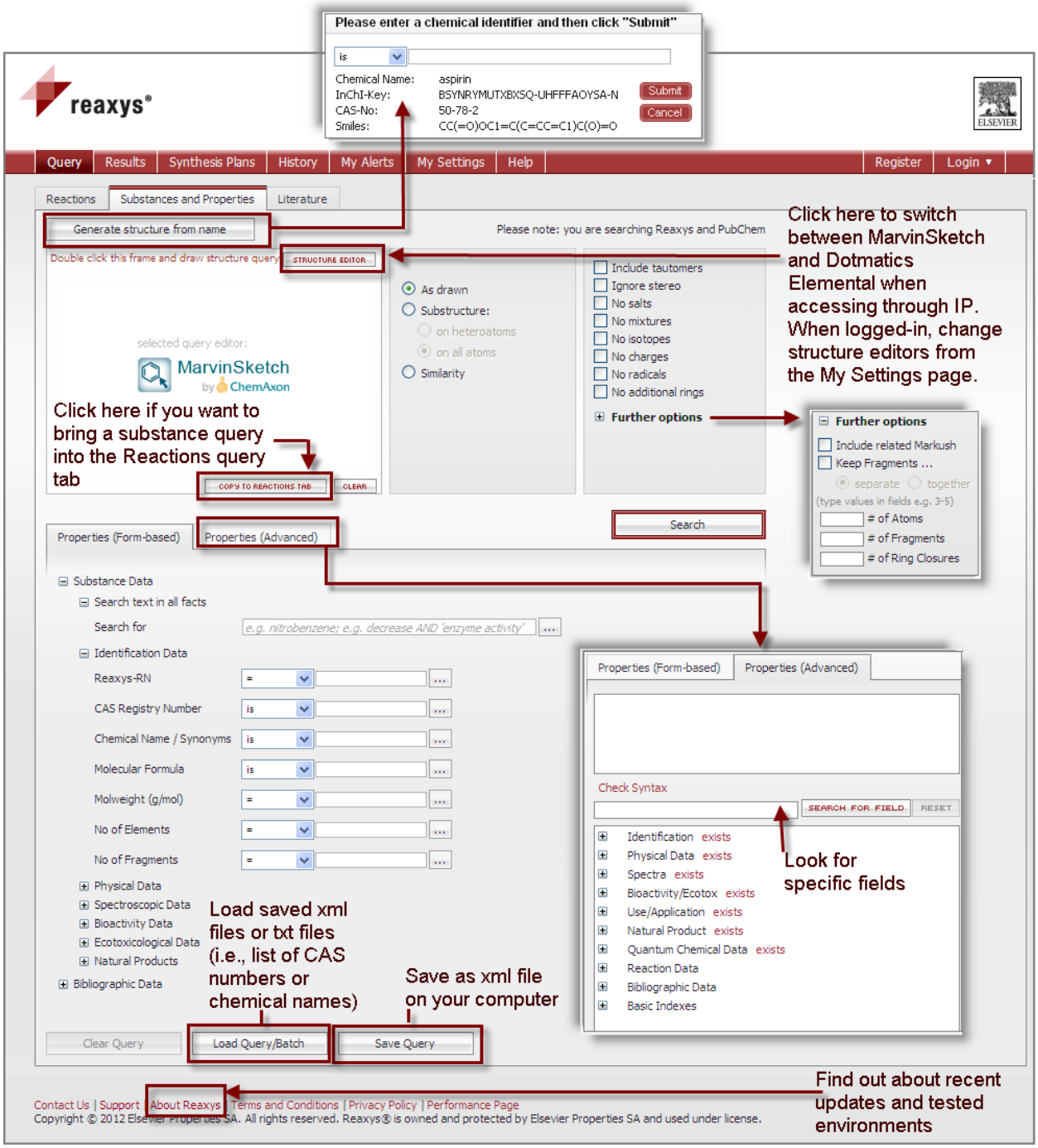
Searching by **formula** is less preferred than by structure because a formula search can be very broad and might result in a large number of hits. Searching with a very specific formula is preferred over searching with formula ranges or searching with wildcards.

Searching by **Ligand formula** will yield relevant results, but new Reaxys users may prefer using a structure, name, or formula search at first.

Please don't forget the **Reaxys Help** file. This contains information such as tips for using Reaxys with different **structure editors** and details about the **Reaxys Generics**.

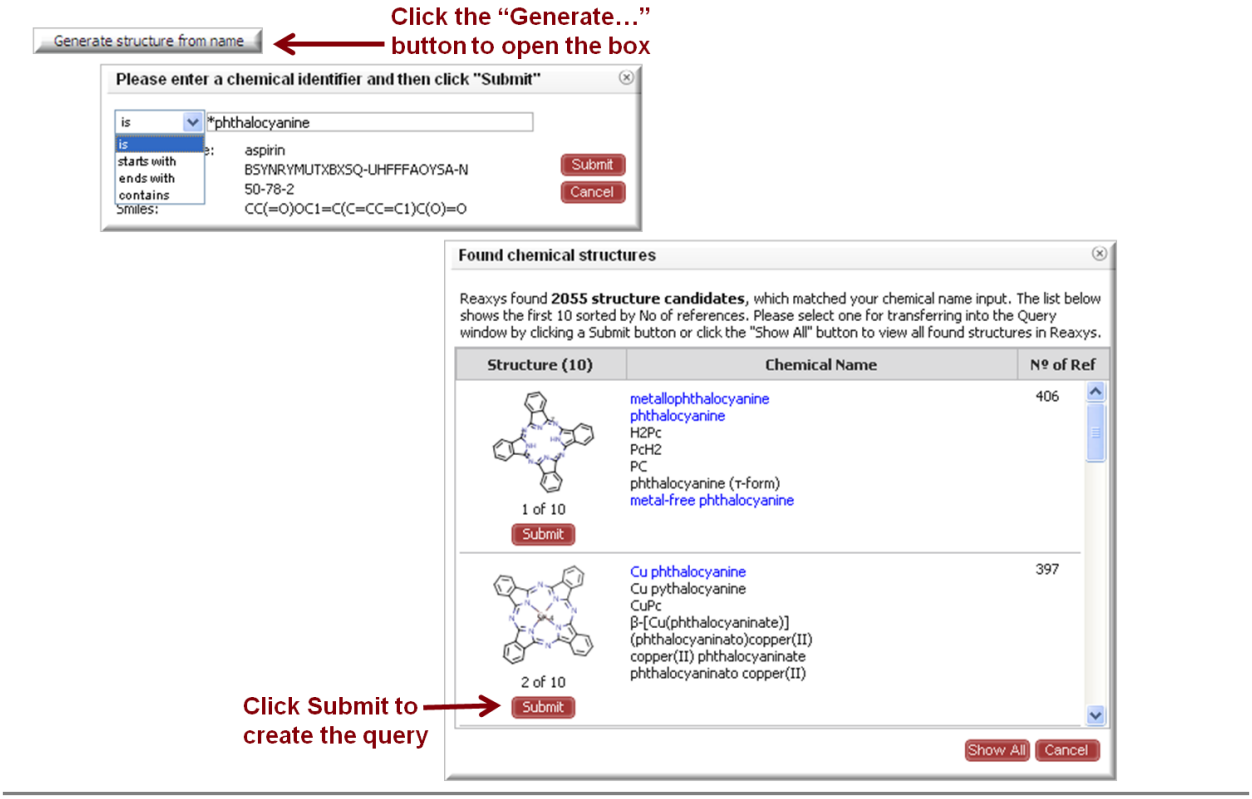






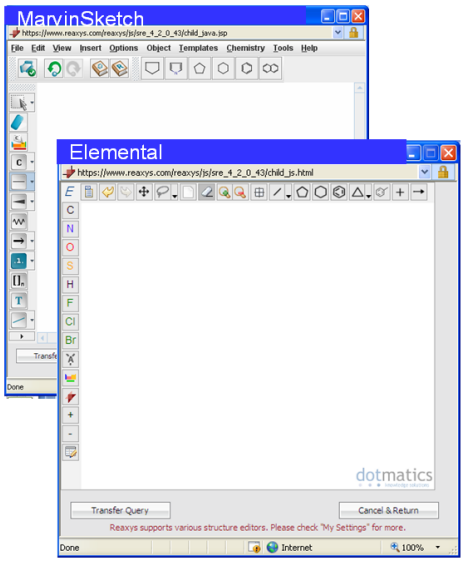
The Reaxys Substance Query page

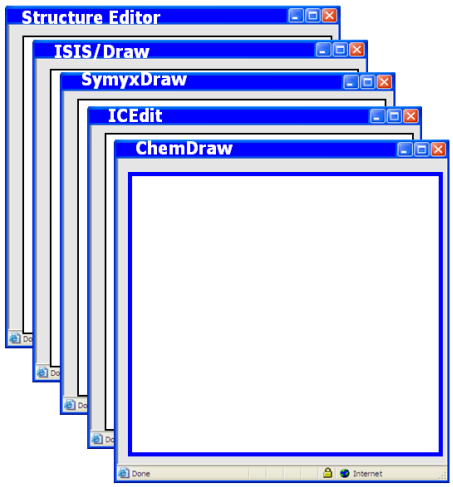
Generate Structure from Name



- **The *Generate Structure from name* functionality** feature enables you to create a query structure without having to draw it.
- You can enter a chemical name (e.g., *zinc phthalocyanine*), a trade/trivial name or abbreviation (e.g., *ZnPc*), a CAS number (e.g., *14320-04-8*), a smiles string, or an InChi key to generate the structure.
- A dropdown menu with the operators *is, starts with, ends with*, and *contains*, along with the wildcard (*), gives you some flexibility when using this feature.
- If several structures are relevant to your entry, a list sorted by **Number of References** appears so that you can select one substance.

Structure Editors

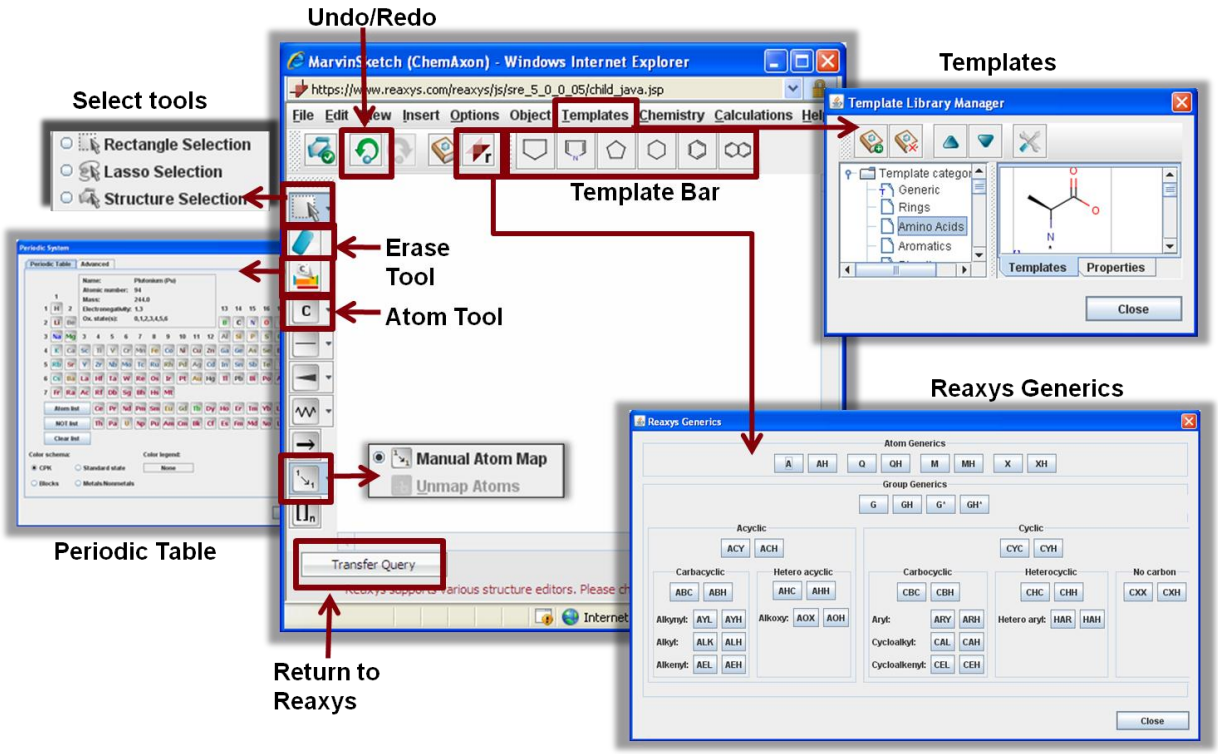




www.reaxys.com/info/support_downloads

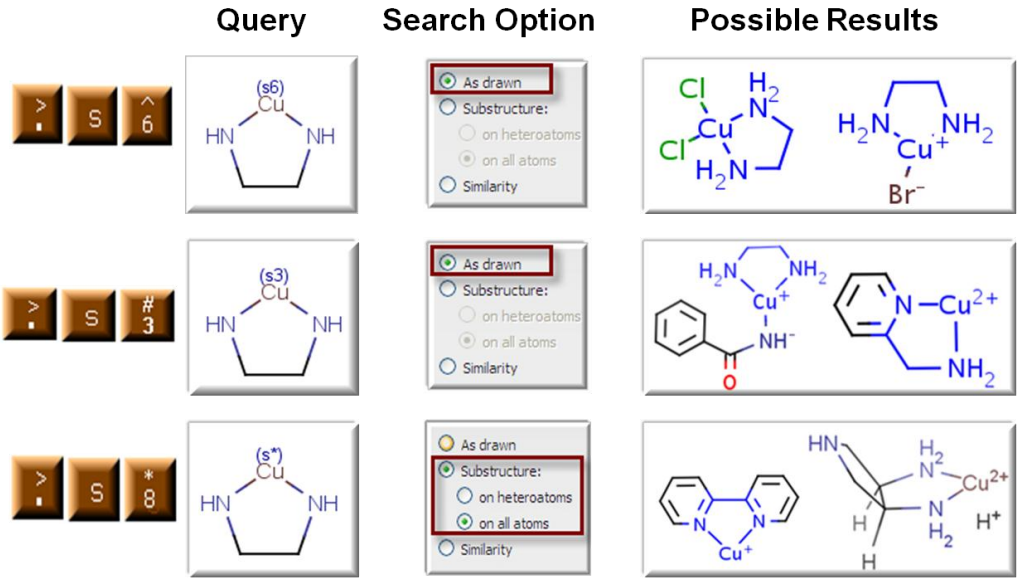
- Structural queries can consist of complete structures or fragments and can contain **atom** and **bond** query features.
- There are 2 structure editors that come with Reaxys and require no installation: MarvinSketch and Elemental, shown on the left.
- Reaxys can also be used with the 5 structure editors shown on the right. Connection software is required and can be downloaded from the Reaxys infosite. www.reaxys.com/info/support_downloads.
- **MarvinSketch** will be used for the examples in this document.
- Consult the **Reaxys Help file** for more drawing tips.

MarvinSketch



- Frequently used tools are show above.
- Right-clicking an atom, bond, or in the white space will display different menus.
- Both the **Rectangle Selection** tool and the **Lasso Selection** tool will select an atom, bond, or the whole structure.
- The **Structure Selection** tool will only select the entire structure.
- There are 2 ways to change the size of the display using the menus: **Options>Zoom** and **View>Transform>Zoom.**
- To **Move** a structure, first select it, then hover over it until you see a **blue box**, and then drag with the mouse.
- To **Rotate** a structure, first select it, then hover over it until you see a **blue pinwheel**, and then drag with the mouse.

Managing Substitution

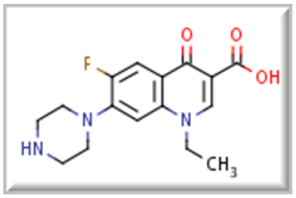


Use Substitution Counts – Find copper diaza compounds by specifying the allowed **number of substituents** on the copper atom.

- Manage substitution by opening up a site to the maximum number of substituents or to a specific number of substituents. Substitution can also be blocked at a specific site.
- **Maximum free sites** – This designation will retrieve ***up to the maximum number of allowed substituents*** on an atom. Use the **Lasso** select tool, click the atom and then type **.-s-6** from the keyboard (in succession, not simultaneously). Set the **Query Options** to **As Drawn** in Reaxys.
- **Specific number of free sites** –In the example above, the atom labeled ***s3*** meaning it can have a maximum of 3 substituents. The copper already has 2 substituents (the 2 N's), so choosing ***s3*** with result in substances with 1 additional substituent (or possibly, no additional substituents). To do this use the **Lasso** select tool to click the atom and then type **.-s-3** from the keyboard. Set the **Query Options** to **As Drawn** in Reaxys.
- **Prevent Substitution at a specific site –** Retrieve substances with substitution anywhere **except** on a specified site. Use the Lasso Select tool, click the atom and then type **.-s-*** from the keyboard . Set the **Query Options to Substructure on all atoms.**

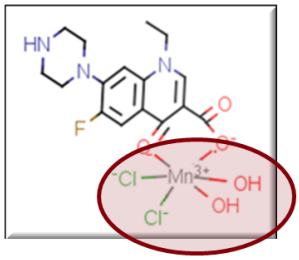
Atom Lists

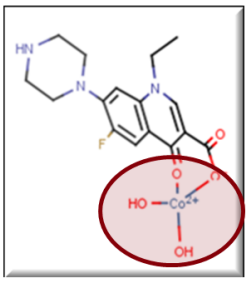
More button
(Periodic Table)

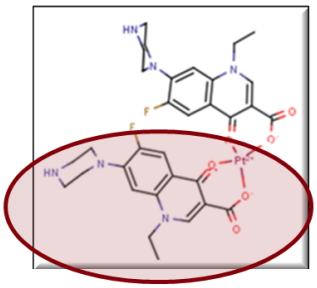


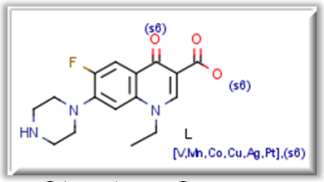
Norfloxacin

[Mn, Co, Pt, V, Cu, Ag]

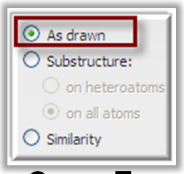




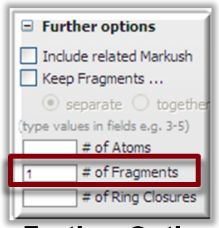




Structure Query



Query Type

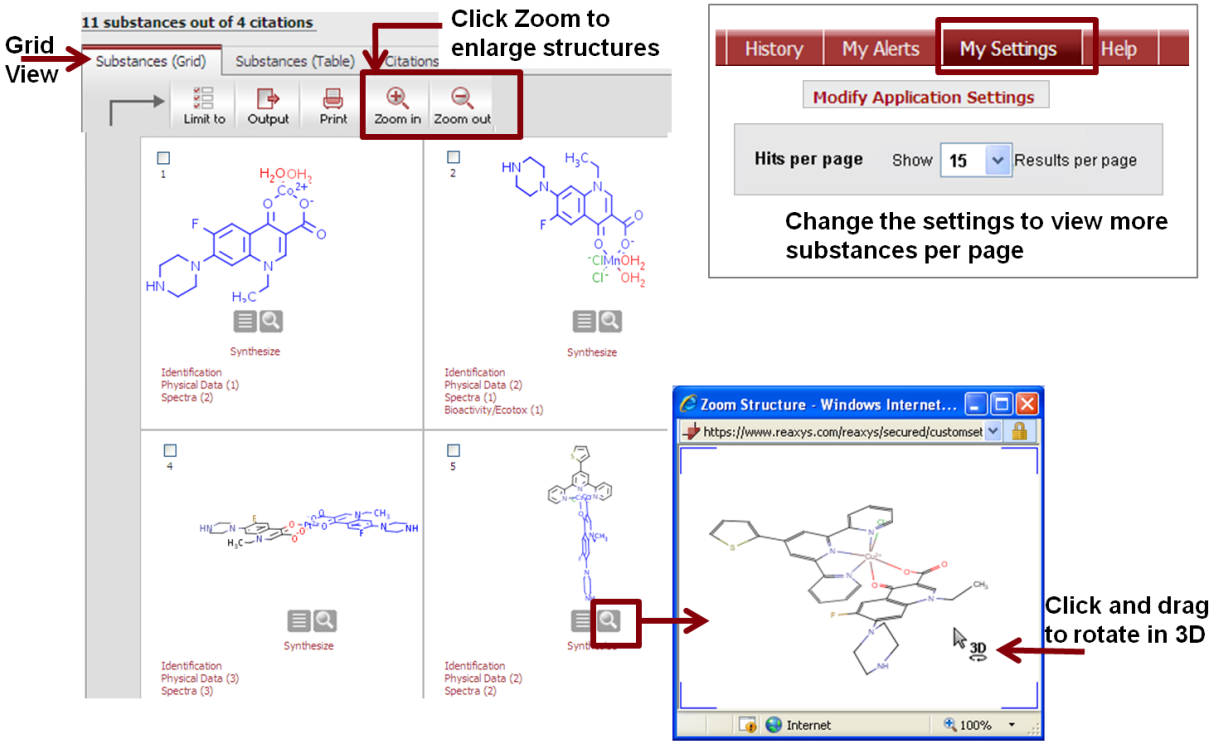


Further Option

Use Atom Lists – Find **coordination complexes** of the antibiotic **Norfloxacin,** limiting the metals to **Mn, Co, Pt, V, Cu, and Ag** using an **Atom List** fragment .

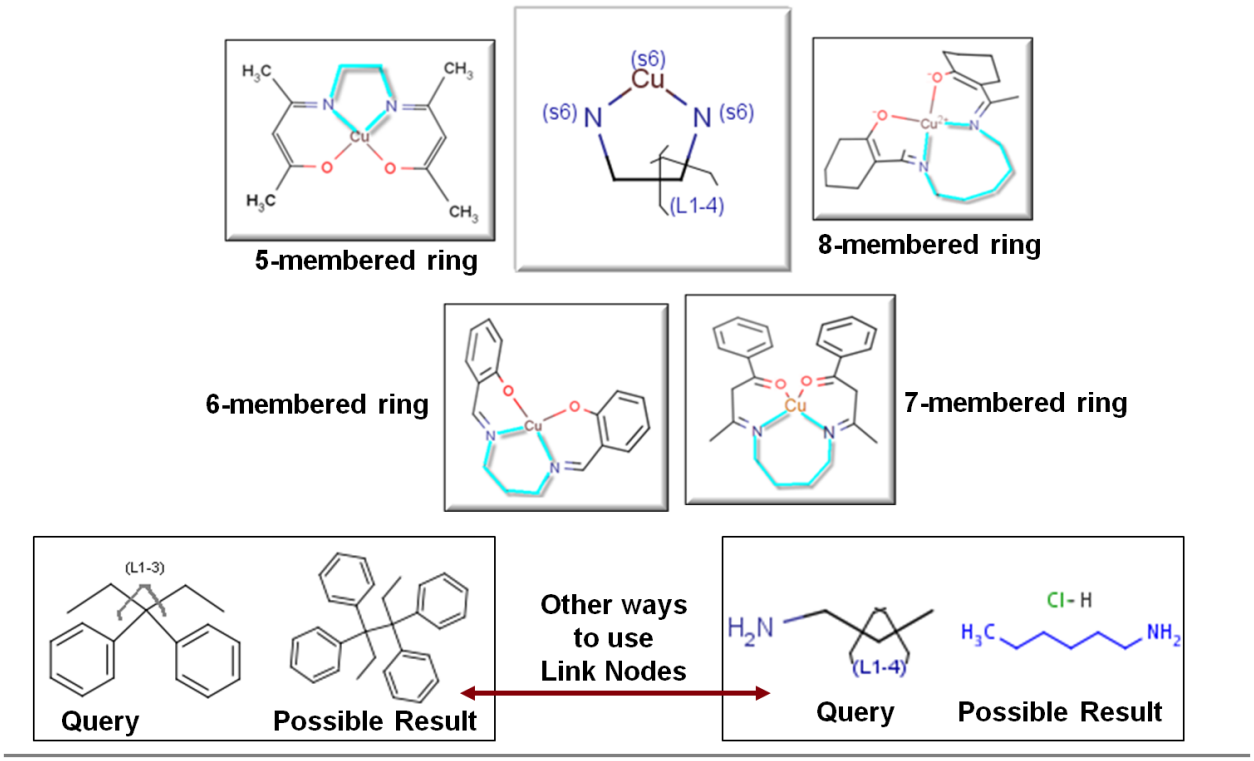
- **Atom lists** can be used to to *include* or *exclude* certain atoms on a certain site.
- **Atom Lists** can replace an atom, or a list can stand on it's own as a separate fragment.
- Draw the structure for Norfloxacin (or use **Generate Structure from Name**). Use the **Template Bar** to draw the rings. Add the appropriate atoms and bonds.
- Create the **Atom List**: Select the **More** button, click **Atom List** to include atoms(Use the **Not** button when you want to exclude atoms).Select **Mn**, **Co**, **Pt**, **V**, **Cu**, **Ag** from the table. Click **Close**.
- Open substitution on the **4-oxo**, the **OH** of the carboxy and on the **list** by clicking in the white space and typing .-s-6 from the keyboard, and then clicking the appropriate atoms.
- Click the **Transfer Query** button in **MarvinSketch.**
- Select options for **Query Type** and **Number of Fragments** in Reaxys: click **As Drawn.** Click **Further Options**link. Type 1 in the box for **Number of Fragments**. Click **Search**

Viewing Results



- The results appear in **Table** view by default. Click the tab for **Grid** view to see substances without details.
- Substances are displayed with 9 per page by default. Change this by clicking the **My Settings** button and selecting **Modify Application Settings** and then changing the number next to **Hits per page**.
- You can enlarge the substance display by clicking **Zoom**.
- You can view a substance in **3D**: most organometallic and coordination compounds can be viewed in Reaxys by simply clicking the **magnifying glass** under a substance and then dragging the mouse in the **Zoom** box.
- If you find a structure that is not displayed in 3D in the zoom box, you can generate the 3D display by right-clicking near the zoomed structure and selecting **Structure>Clean 3D.**

Link Nodes



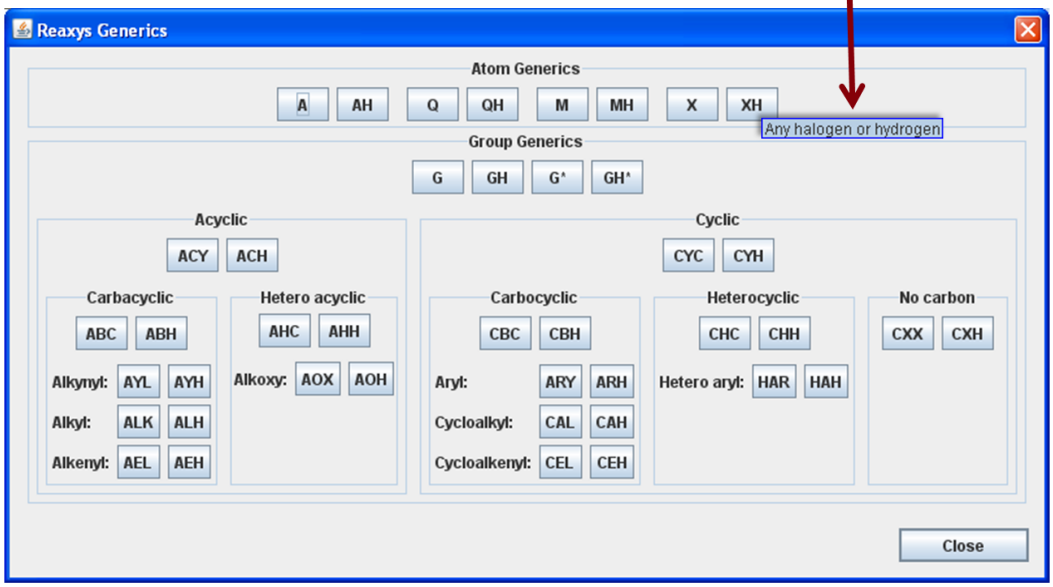
Use Link Nodes – Find **copper diaza rings** of **varying size** using **Link nodes.**

- **Link Nodes** are used to define repeating units.
- The units can be rings or chains.
- The **Link Node** is the atom that is selected. Anything within the brackets of the **Link Node** will be repeated.
- Create the copper diaza query above. Use the **As Drawn** query option in Reaxys.

Reaxys Generics

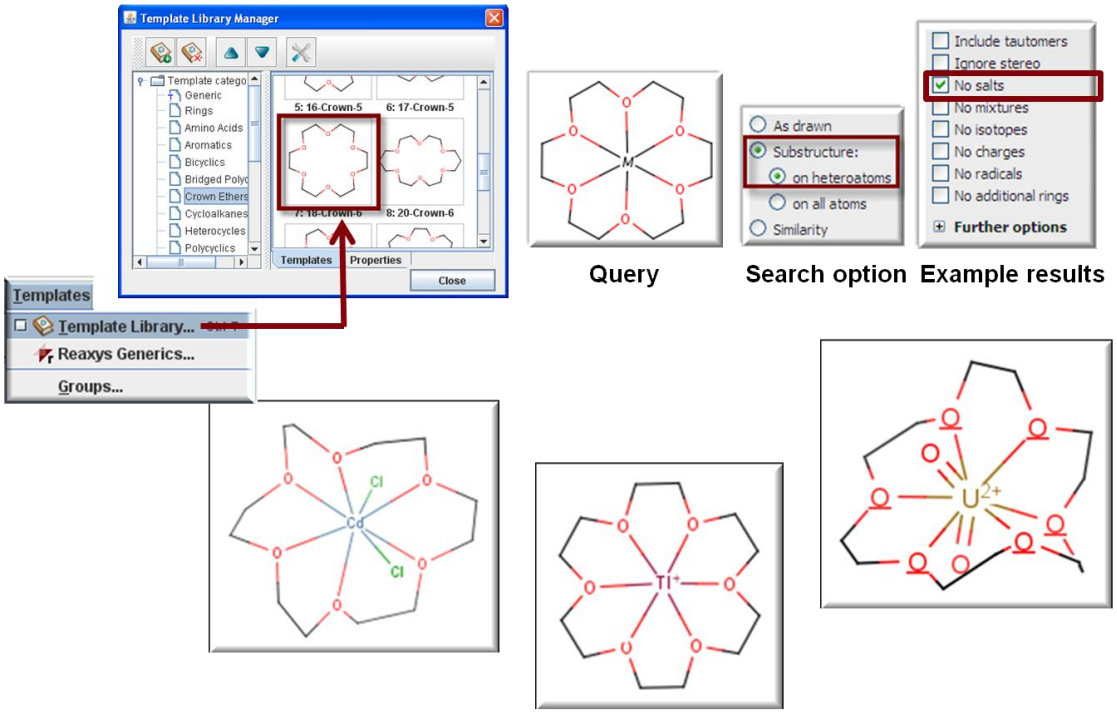
Click the "r" in MarvinSketch to access the Generics

Hover over a group to see the definition



- The **Reaxys Generic Groups** provide you with abbreviations so that you can generalize your queries.
- The Generics are divided into **Atom Generics** and **Group Generics**.
- All symbols ending in "**H**" allow for hydrogen in addition to the defined **atom** or **group**. For example, ALK is the abbreviation for an alkyl group. The abbreviation ALH would allow an alkyl group or a hydrogen atom.
- The groups are hierarchically ordered starting with **G** as any group.
- G* and GH* are the only generics that allow ring closure at the site.
- For detailed information, consult the **Reaxys Help** file.
- G and G* can have multiple attachment points to the structure. Other predefined generic groups can have only one attachment point to the structure.
- Predefined generic groups can only have one bond to the parent structure.

Use Templates and Generics

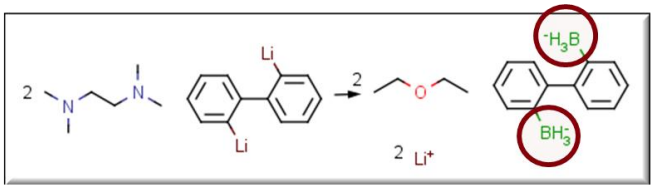


Use Reaxys Generics and **Templates** - Find coordination compounds of 18-crown-6 ethers using **Reaxys Generics** and **templates**.

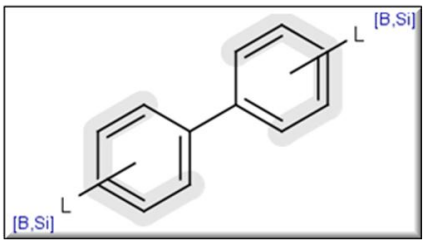
- For the example above, follow these steps:

1. Select **Templates>Template Library**, click **Crown Ethers** in the list, and select the template for **18-crown-6**. Click **Close**.
2. Click the "**r**" to open the **Generics**, select **M**, click **Close**, and click in the middle of the crown ether.
3. Use the **Single Bond** tool to connect the oxygens to the metal.
4. Click the **Transfer Query** button in **MarvinSketch**
5. In Reaxys, set the **Query Options** to **Substructure on heteroatoms** and check the box for **No Salts**.
6. Click **Search.**

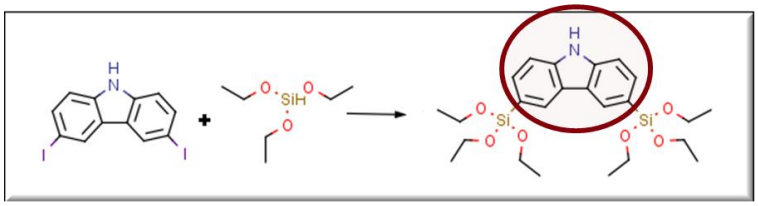
Position Variation Bond



Find preparations with boryl or silyl substitution anywhere on the ring



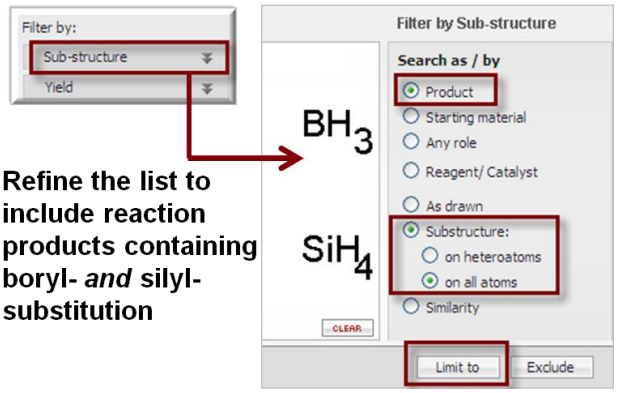
Eliminate preparations with ring closure around the core

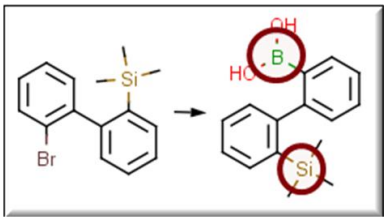


Use Position Variation Bond – Find preparations for **biphenyl** compounds **with boryl- and silyl substitution** anywhere on the rings using the **Position Variation bond.**

- The **Position Variation bond** is used to allow specific substitution on a ring without specifying the exact location on the ring.
- The substitution can be left as a carbon or changed to another atom, a functional group, a list of atoms, or a ring. Use substitution labels as described on **pg 8**.
- To apply the **Position Variation bond**, use the **Lasso Select** tool to encircle the relevant atoms, right-click in the white space, and select **Edit Structure>Add>Position Variation bond**.
- For the example above, draw the biphenyl, apply the **Position Variation bonds**, and add an **atom list** for **B** and **Si** to the bonds. Transfer the query to **Reaxys**. If your query appears in the **Substance Query tab**, you can copy it to the **Reactions tab** by clicking the **Copy to Reactions tab** button below the structure.
- In the **Reactions Query tab**, select **Substructure on all atoms** and put a check in the box for No Additional Rings (this prevents ring closure around the core).

Filter by Substance

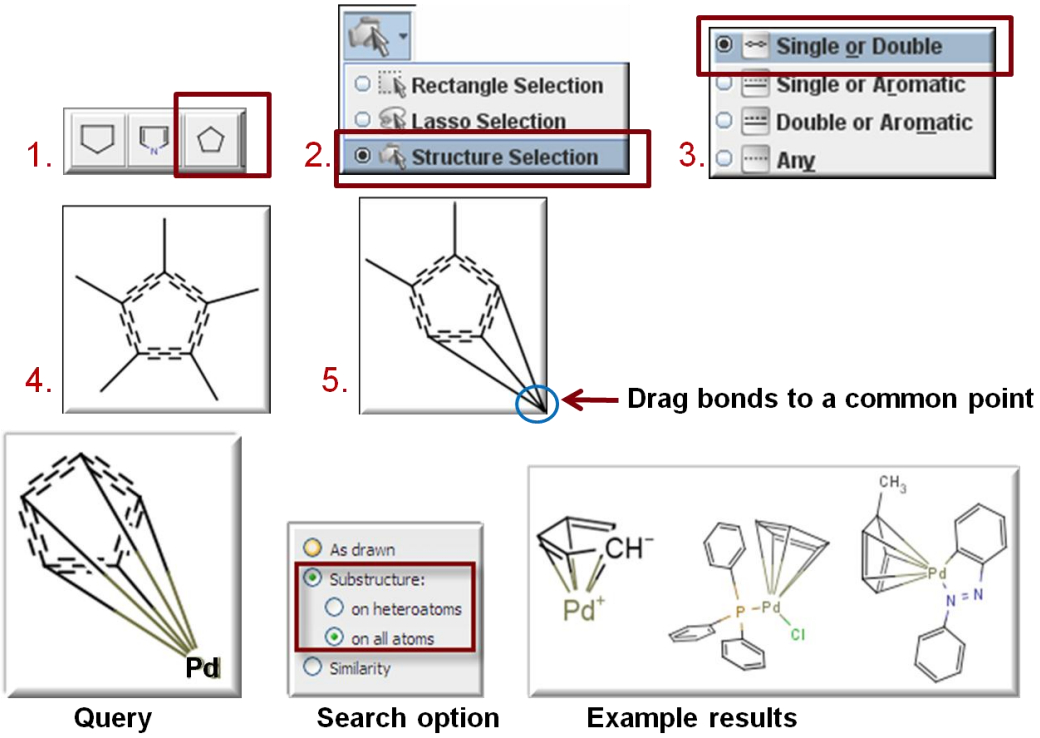




Use the Substructure Filter – Filter the list to include only reactions with products that contain both **boryl-** and **silyl-** substituents using the **Substructure Filter**. Save the list.

- About 251 reactions were retrieved in the previous search. Do any of these reactions have products containing both **boryl- and silyl-** substituents? You can filter a list by structure to include or exclude elements or structures.
- Click the filter for **Substructure**.
- To add **B** and **Si** to the filter box, double click the structure box to open **MarvinSketch**.
- Click the **More** button to access the periodic table. Click **B**. Click **close**, then click in the white space. Repeat with **Si**. Transfer to the filter box by clicking **Transfer query**.
- In the filter box, select **Product** and **Substructure on all atoms**. Click **Limit to**.
- About 11 reactions are retrieved. Notice the **Breadcrumbs** at the top. If you want to return to the unfiltered list, click the breadcrumb with 251 reactions.
- Save lists by clicking the **History** button at the top. Click the link for **Store**.

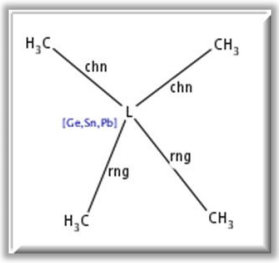
Bond Type



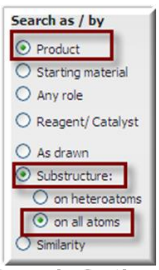
Use Bond Type – Find cyclopentadienyl-palladium complexes using **Single or Double Bonds** on the **Cp** ring to ensure that no substances are missed.

- Bonds can be designated as several types of bonds, such as **Any Bonds**, and **Single or Double Bonds**. Reaxys will retrieve hits with only that type of bond.
- Different **Bond Types** can be used multiple times in one query.
- For the example above: **1**. Click the **cyclopentane template**. **2.** Use the **Structure Selection** tool to select the ring. **3**. From the **Object** menu, select **Bond>Type>Single or Double.** **4.** Use the **Single Bond tool** to add 5 bonds to the structure. **5.** Use the **Lasso Select tool** to click and drag each bond to a common point. **6.** Click the **More** button, select **Pd**, click **Close**. Click the common point of the structure.
- Click the **Transfer Query** button in **MarvinSketch.**
- Set the **Query Options** to **Substructure on all atoms** in Reaxys

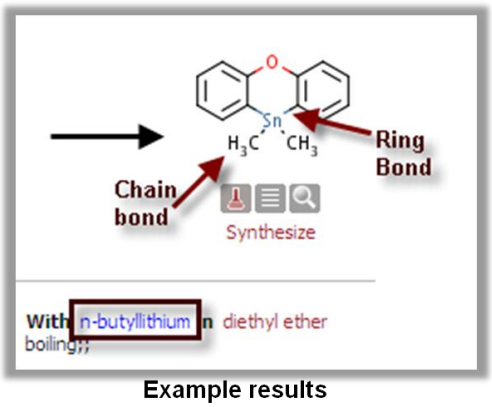
Bond Topology



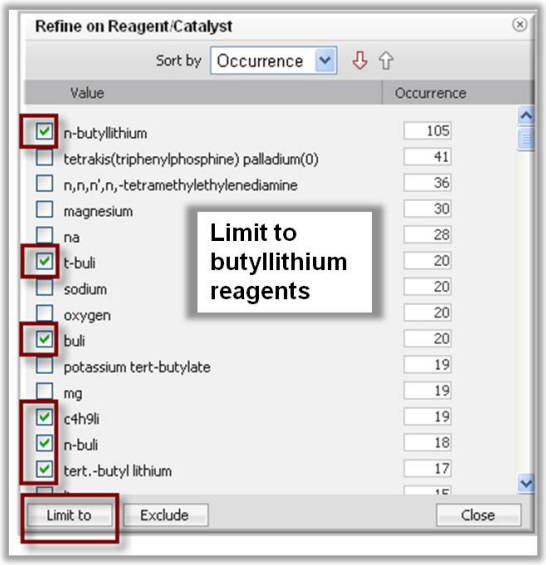
Query



Search Options



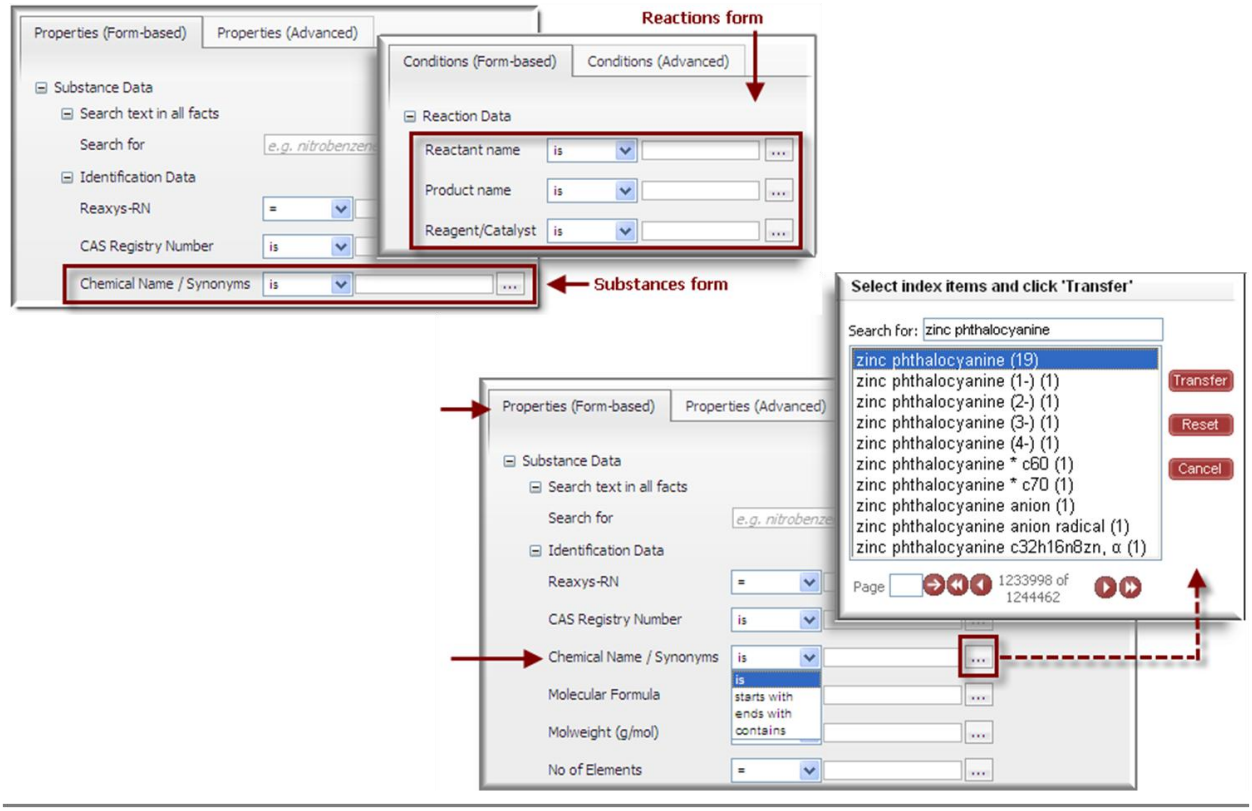
Example results



Use Bond Topology – Find preparations of organometallic compounds with **butyllithium** as the catalyst. Designate bonds as being part of a ring or part of a chain using **Bond Topology.**

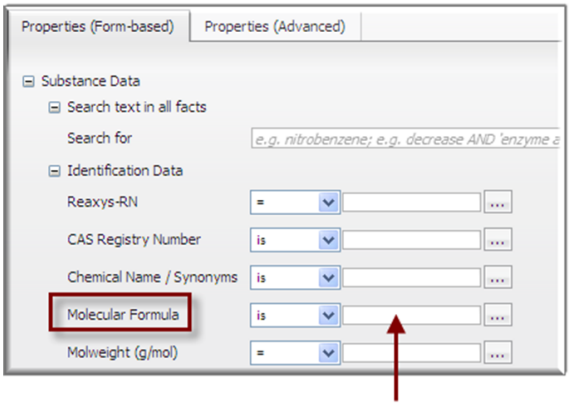
- **Bond Topology** is a convenient way to generalize part of a query.
- For the example above: **1**. Draw the core structure using the **Single bond** tool. **2.** Use the **Lasso Select** tool to encircle 2 of the bonds to select them. From the **Object** menu, select **Bond>Topology>Ring**. **3.** Select the other 2 bonds. From the **Object** menu, select **Bond>Topology>chain**. **4.** Select the middle "**C**" **atom** and then click the **More** button. Click **Atom List** and select **Sn, Pb**, and **Ge**.
- Click the **Transfer Query** button in **MarvinSketch.**
- Set the **Query Options** to **Product** and **Substructure on all atoms** in Reaxys**.** Click **Search.**
- **In the results, click Filter by Reagent/Catalyst.** Click the **More link** at the bottom of the filter box, and then select the relevant **Li-containing reagents**. Click **Limit to**.

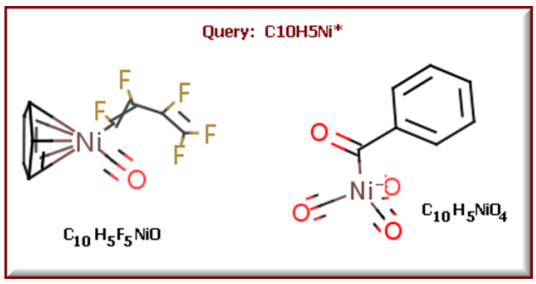
Use the Chemical Name field

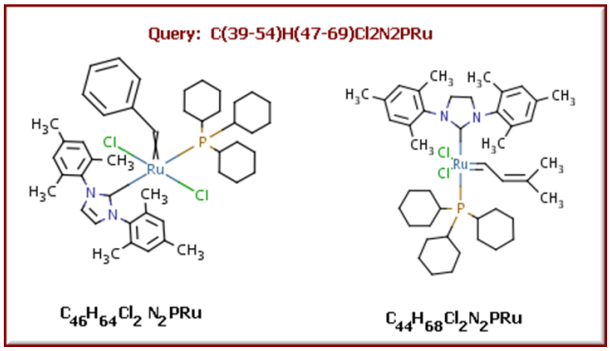


- The *Chemical Name* field can be queried from the **Properties (Form-based)** tab on the **Substances** query page and from the **Conditions** tab on the **Reactions** query page (*Reactant Name*, *Product Name, and Reagent/Catalyst name*).
- A dropdown menu with the operators *is, starts with, ends with*, and *contains*, along with the wildcard (*), gives you some flexibility when using the **Name** fields.
- Alternatively, click the grey box to open the index. From the Index, you can type a word, select the appropriate word or words from the list (use the **control** or **shift** key), and then click the **Transfer** button.

Search by Molecular Formula

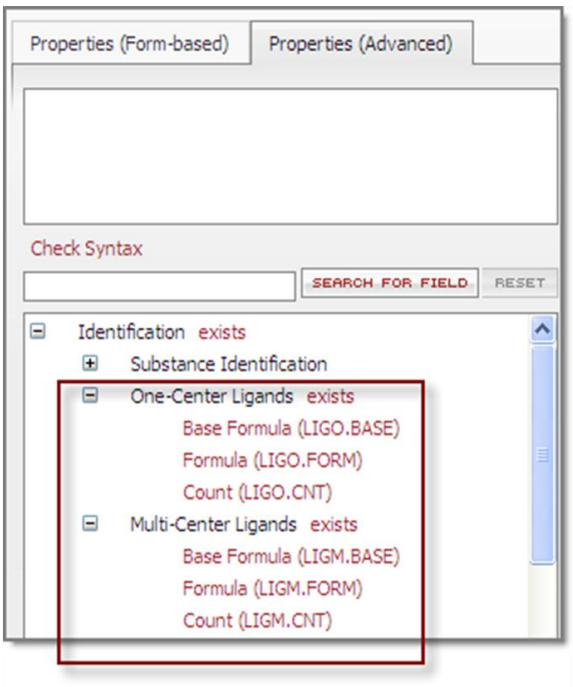


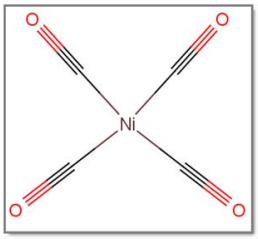




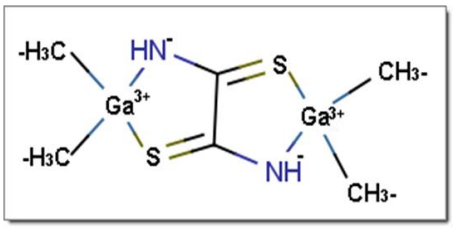
- The *Molecular Formula* field can be queried from the **Properties (Form-based)** tab on the **Substances** query page. Type the formula into the box*.
- It is not necessary to write the formula in Hill order.
- An element without a number is assumed to have a quantity of one.
- Use **Ranges** or a **Wildcard** when needed.
- Though “C”, “H”, and some elements may be written in either upper case or lower case, other elements must be written with the first letter in upper case and the second letter in lower case. For example lower case “ni” will be interpreted as nitrogen and iodine, but when it is written as “Ni” it will be interpreted as nickel.
- *Alternatively, click the grey box near the molecular formula box to open the index. From the index you can type, select the appropriate formula or formulas from the list (use the **control** or **shift** key), and then click the **Transfer** button (as shown in the previous chapter)

Ligand Search Fields





One-center ligand



Multi-center ligand

- The ligand fields are divided into **one-center ligands** and **multi-center ligands**. A **one-center ligand** has at least one non-metal atom bound to one metal atom. A **multi-center ligand** has at least 1 non-metal atom bound to at least 2 metal atoms.
- Multi-center ligands are indexed in Reaxys as both multi-center ligands and as individual one-center ligands.
- These fields are powerful tools for finding ligand- metal complexes.
- They are different from the other molecular formula fields in Reaxys because they use **Ligand Codes**, rather than element symbols.

Ligand Codes

Use these field codes when setting up your queries

Code	Atom(s)					
L	C					
A	B	Si	Ge			
D	N	P	As	Sb		
Q	O	S	Se	Te		
X	H	F	Cl	Br	I	At

There are also "special" ligand fields

Code	CO	CS	CN	CNS	CNO	CNR*

- Each type of ligand can be searched using the fields: **Base Formula, Formula, Count**.

Base formula – This is the abstract formula of the coordination center(s) and all ligand codes of a compound. The ordering of the formula is as follows:

1. all metal centers (ordered alphabetically)
2. the ligand codes are ordered in the following manner:
   A, CN, CNO, CNR, CNS, CO, CS, D, L, Q, X
3. within the same ligand types, they are ordered on ascending denticity and the frequency is not taken into consideration

Formula – the ligand formula field contains the ligand codes which describe the elements (in groups) and the number of the atoms that are connected to the central metal atom(s). A ligand formula is given for all structured compounds or fragments which contain at least one metal atom and at least one coordinating ligand atom of the classes "L, A, D, Q, X" or a special ligand (for special ligands, the substituent R has no further bond to metal atoms). The denticity of a ligand is put in parentheses in front of the ligand code. If a ligand is described by >1 code, they are ordered alphabetically and the denticity of the code is put in parentheses in front of the code.

Count – the frequency of a certain ligand within the compound is indexed in this field.

Note: The ligand formula field(LIGO.FORM) describes only the denticity of the ligand not the connectivity to the metal center(s).

Ligand Fields Search Examples

Examples:

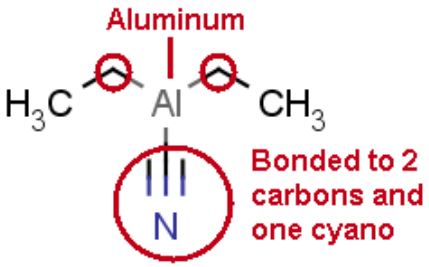
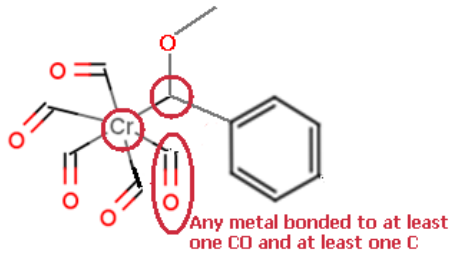
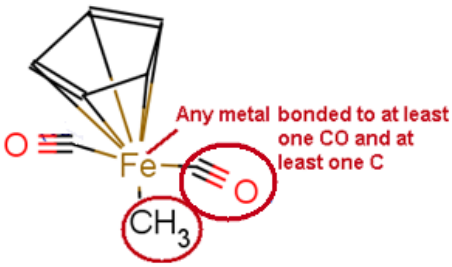
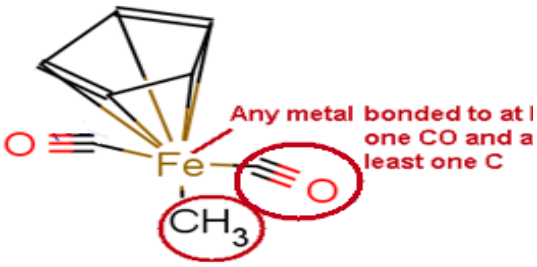
Search for:	**Use this:**
hexa carbonyl chromium	Cr{CO} 6
tetra halogeno palladium compounds	Pd{X}4
nickel complex with two tridentate ligands connecting by one pnictide and two chalcogenide atoms	Ni{D(2)Q}2

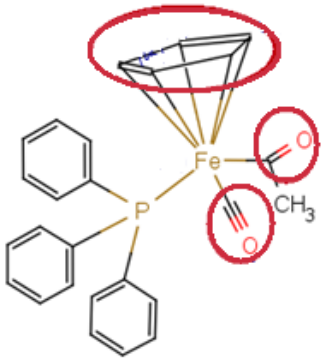
Examples:

Search for:	**Use this code:**
halogenid or hydride ligand µ-halogenide or µ-hydride ligand	**X**
ligand connecting by two halogenide or hydride atoms e.g. η^2-hydrogen, η^2-BH4	**(2)X**
(monodentate) carbonyl	**CO**
ligand connecting by C and chalcogen e.g. µ-η^2-carbonyl (by C and O)	**LQ**
Ligand connecting by four pnictide Atoms e.g. porphyrins, phthalocyanines, tetraaza-cyclam	**(4)D**
ligand connecting by five C atoms to one or more metal centers e.g. η_5-cyclopentadienyl	**(5)L**
ligand connecting to metal(s) by C e.g. µ-carbonyl (only by C), bridged alkyl-, η^2 alken-, η^2-alkin ligands	**(2)L**

The hit sets will contain mono - as well as poly-nuclear complexes.

Ligand Fields Search Examples, continued…

Query	Example Result
1. Find substances where aluminum is bonded to 2 carbons and a CN **Query is** LIGO.BASE = 'Al{CN}{l}2'	
2. Find substances where any metal is bonded to at least one C and at least one CO. **Query is** LIGO.FORM = 'l' AND LIGO.FORM = 'co'	 
3. Find substances where iron is bonded to a five-membered carbon ring, 2 CO's, and one C. **Query is** LIGO.BASE = 'Fe{(5)L}{CO}2{L}'	

Query	**Result**
4. Find substances where iron is bonded to at least one CO, at least one C, and also bonded to anything else. **Query is:** LIGO.BASE = 'fe*' AND LIGO.FORM = 'l' AND LIGO.FORM = 'co'	

Practice Exercises

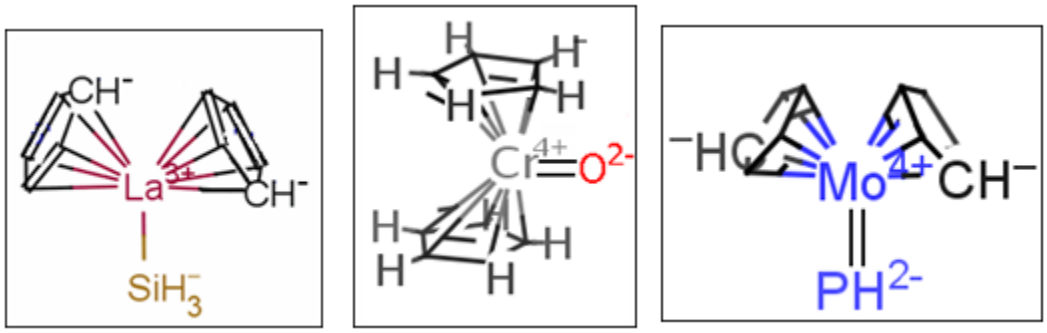
I. Use **Generate Structure from Name** to find the structure for potassium ferrocyanide, selecting the structure with the greatest number of references for your query. Run the search using “As drawn” as the search type. View the result in 3D. Use the animation feature to rotate the structure.

II. Use the **Chemical Name** field to find all substances with *bromoferrocene* in the name.

III. Use the **Chemical Name** field to find *ferrocene carboxamide, ferrocene carboxaldehyde,* and *ferrocene methylamine* with one query, keeping in mind that these chemical names can also be spelled without the space between words.

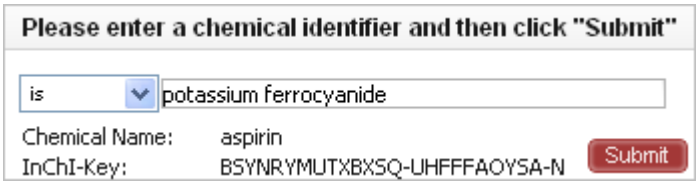
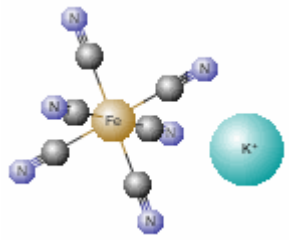
IV. Use the **Molecular Formula** field to find substances containing cobalt, 10-15 carbons, 10-30 Hydrogens, 1-3 Nitrogens and anything else.

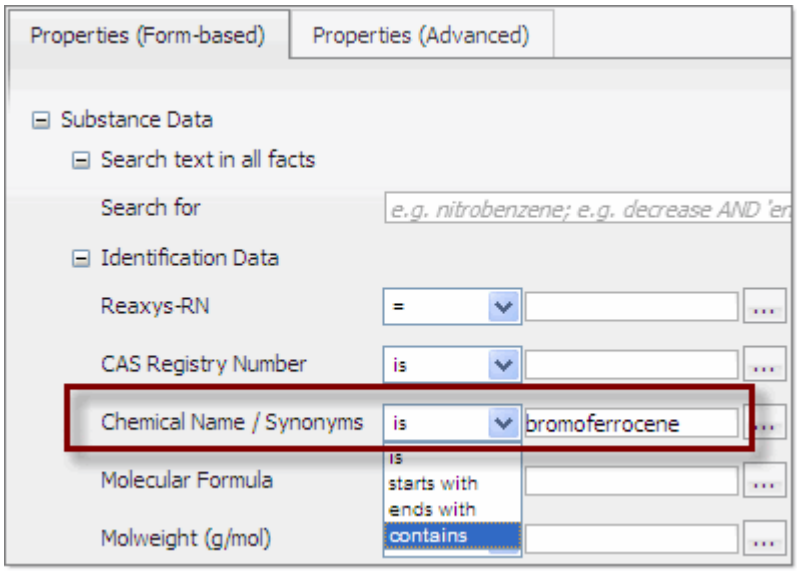
V. **Draw a query with 2 cyclopentadienyls** that will include the 3 substances below in the results. Draw the parent and use atom and bond query features as needed.

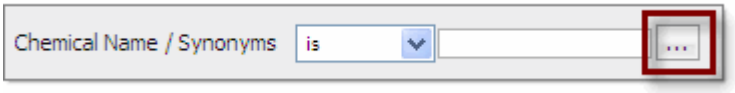
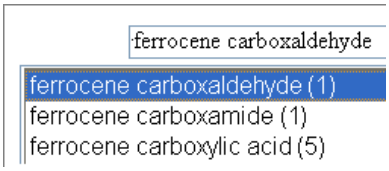
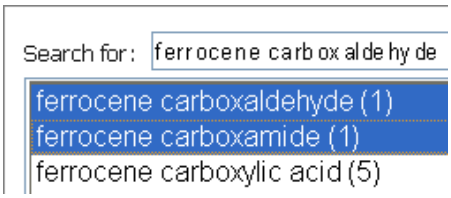
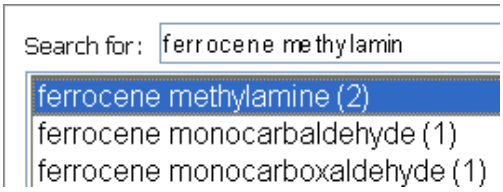
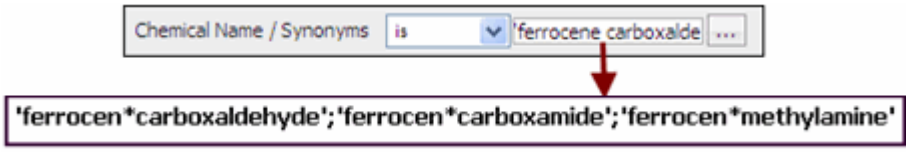


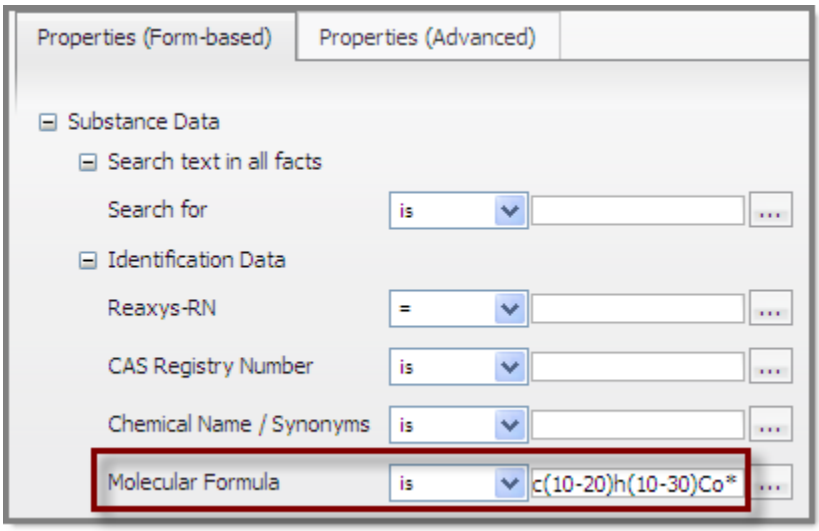
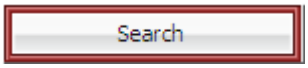
VI. Draw a query to retrieve **Grubb’s Catalysts**.

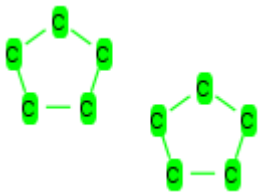
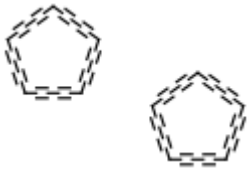
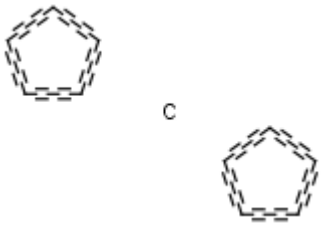
VII. Find coordination complexes involving the heteroatoms of Salen and a metal. Allow a substituted methyl to appear on any location of the 2 rings

	Use **Generate Structure from Name**
Exercise 1	Find the structure for potassium ferrocyanide, selecting the structure with the greatest number of references for your query. Run the search using “As drawn” as the search type. View the result in 3D. Use the animation feature to rotate the structure.
	1. Click the **Generate Structure from Name** button.
	2. Type potassium ferrocyanide. Click **Submit**. 
	3. Click **Submit** under the first structure in the list.
	4. Click **Search**
	5. Left click the magnifying glass.
	6. Drag with the mouse to move the structure.
	7. Right click and select **Animation> Play**. To control the **angle** and **speed** of the animation, click and drag the mouse near the structure. You can drag quickly or slowly and in different directions. To change the look of the molecule, select **Display** 

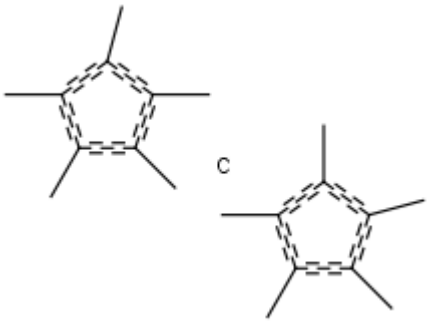
	Use the **Chemical Name** field
Exercise II	Use the **Chemical Name** field to find all substances with *bromoferrocene* in the name.
	1. Type *bromoferrocene* into the **Chemical Name** field on the **Properties (Form-based)** tab. Select *contains* from the dropdown menu. 
	2. Click **Search**

	Use the **Chemical Name** field
Exercise III	Use the **Chemical Name** field to find *ferrocene carboxamide, ferrocene carboxaldehyde,* and *ferrocene methylamine* with one query, keeping in mind that these chemical names can also be spelled without the space between words.
	1. Click the grey box next to the **Chemical Name** field on the the **Properties (Form-based)** tab. 
	2. Type *ferrocene carboxaldehyde* into the box. Click on this name in the list. 
	3. *Ferrocene carboxamide* appears below *ferrocene carboxaldehyde*. Hold down the **shift key** and click *ferrocene carboxamide*. 
	4. Type ferrocene methylamine. Hold down the **Control key** and click *ferrocene methylamine*. Click the **Transfer** button. 
	5. Edit the query to include wildcards as shown below. 

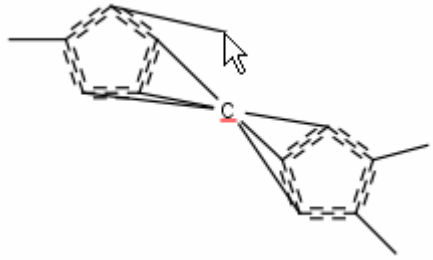
	Use the **Molecular Formula** field
Exercise IV	Use the **Molecular Formula** field to find substances containing cobalt, 10-15 carbons, 10-30 Hydrogens, 1-3 Nitrogens and anything else.
	1. Type the following into the **Molecular Formula** field on the **Properties (Form-based)** tab on the **Substances** query tab: **c(10-20)h(10-30)Co*** 
	2. Click **Search.**

	Draw a Cp query
Exercise V	Draw a query that will include 2 cp rings bonded to either **La, Mo**, or **Cr** in the results. The metal can have one additional ligand bonded to **O, Si**, or **P** via a single or double bond. Draw the parent and use atom and bond query features as needed.
	1. In MarvinSketch, click the **cyclopentane template** and then click in the drawing area twice.
	**2.** Click the **Structure Selection tool** and click an atom in one of the structures. Hold down the **Shift key** and click an atom in the other structure. 
	**3.** Select: **Object>Bond>Type>Single or Double** 
	4. Click the **C Atom tool**. Click in the middle of the 2 structures. 

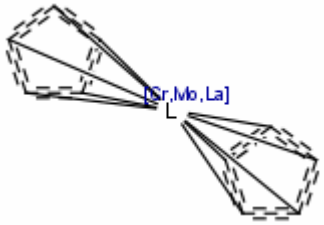
5. Click the **Bond tool** and click an atom in a ring. Repeat until you've added 5 bonds to each structure.

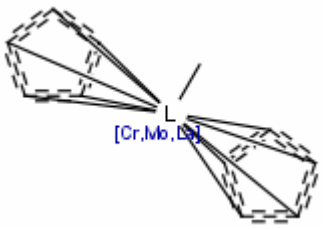
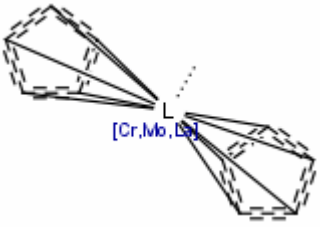
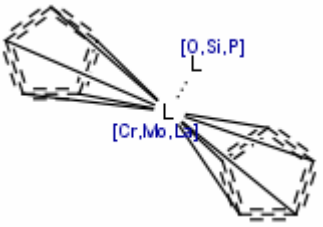


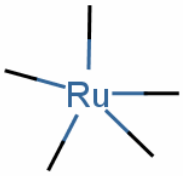
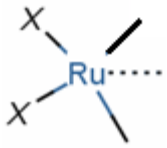
6. Use the **Lasso Select** tool and click an atom on one of the bonds. Drag the bond until it reaches the carbon in the middle of the 2 structures. Repeat with the remaining bonds.

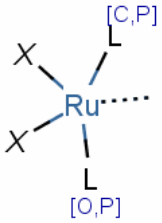
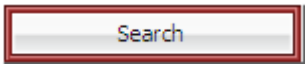


7. Click the **More** button . Click the **Atom List** button and select **Mo**, **Cr**, and **La**. Click **Close**. Then click the **C** in the middle.



	8. Click the **Bond tool** and click the " L" for the Atom List to add the bond. 
 	9. Use the **Select tool** to right click the new bond and then select **Edit Bond>type>Any**. 
 	10. Click the atom at the end of the bond, click the **More** button, and add **P, Si**, and **O** as as in **Step 7**. 
	11. Click **Transfer Query**. Select **As Drawn**, and click **Search**.

	Grubb's Catalysts
Exercise VI	Draw a query to retrieve first and second generation Grubb's Catalysts.
	1. Click the **More** button. Select **Ru**. Select **Close** and then click in the drawing area. 
	2. Click the single bond tool, click the Ru and drag and draw 5 bonds. 
 	3. Use the **Select tool** to right click one of the bonds and then select **Edit Bond>type>Any**. 
	4. Then click the **Reaxys Generics** button, click **X**, and click 2 of the atoms on the structure. 

 	5. Use the **Select tool** to click one of the atoms, click the **More** button, click the **Atom List** button, and select **C** and **P**. Click **Close**. Repeat with the remaining atom, using **O** and **P** as the atom list. 
	6. Click **Transfer Query.** Select **Substructure on All Atoms**, and click **Search.**

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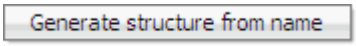
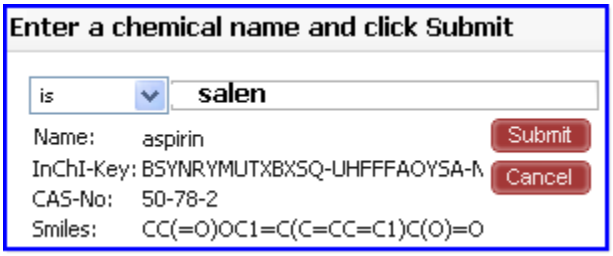
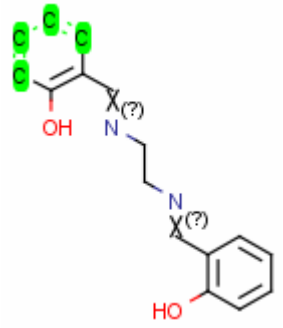
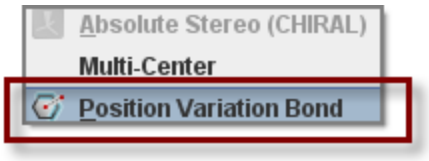
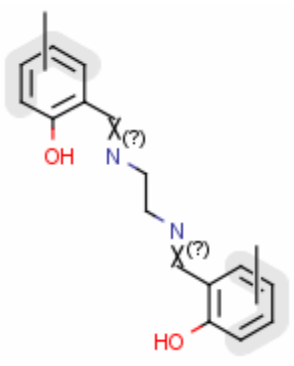
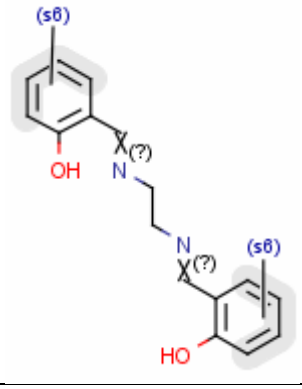
	Find Coordination Complexes
Exercise VII	Find coordination complexes involving the heteroatoms of Salen and a metal. Allow a substituted methyl to appear on any location of the 2 rings.
	1. Click the **Generate Structure from Name** button. Type in *salen.* Click **Submit.** 
	2. Double click in the structure box to open **MarvinSketch**
	3. Use the **Lasso** select tool and select the 4 open atoms. 

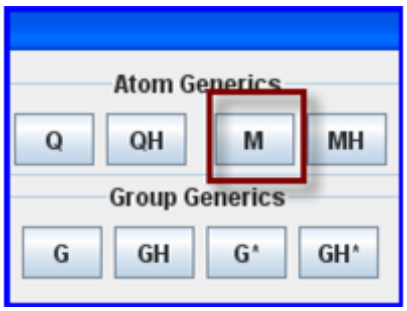


4. **Right click** and select **Edit Structure>Add>Position Variation Bond.** Repeat with the second ring.

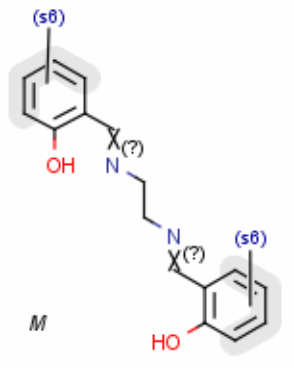


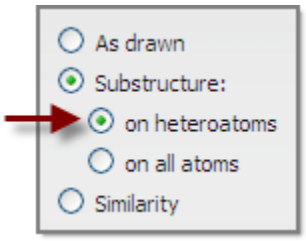
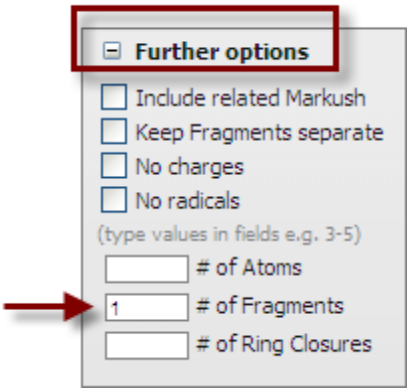
5. Use the **Lasso** select tool and click anywhere in the screen. Type **.S6** (in succession, not together) and then select each methyl.





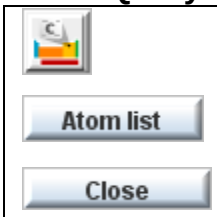
6. Click the **R** button. Select the **M**. Click **Close**. Then click near the structure.



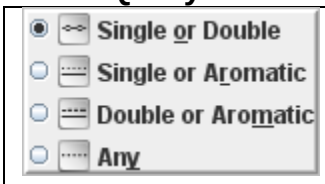
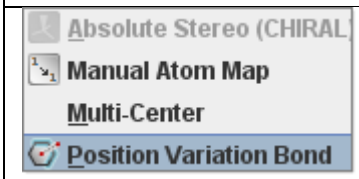
	7. Click **Transfer Query.** Select **Substructure on Heteroatoms**. 
	8. Select **Further Options**. Then type **1** for **# of Fragments**. Click **Search.** 

Quick Reference

Atom Query Features

	**Atom Lists** – To create an atom list, click the **More** button. Then click the **Atom List** button, click the desired elements and the click **Close**. The list will be visibble on the mouse cursor. Click the desired atom in the query to apply the **Atom List.**
	**Allow maximum substitution** – To open a site to substitution whenperforming an **As Drawn** query, click the atom in the query and type **.s 6** (period-s-6). [Type the keys one after the other, not together] (Based on United States keyboard layout)
	**Block substitution** – To block substitution on a site when performing a substructure search, click the atom in the query and type **.s*** (period-s-asterisk). [Type the keys one after the other, not together] (Based on United States keyboard layout)
	**Link Node** – To define a range of repeating atoms, use the **Lasso Select** tool to select the atom to be used as the repeating unit, right-click, and select **Edit Atom>Link Node**. Then select a number.
	**Reaxys Generic Groups –** To use the metal abbreviation, click an atom in the query, click the **R** button, and then select **M**. (For more details about the **Reaxys Generic Groups,** please see the **Reaxys Help file.)**

Bond Query Features

	**Bond type –** To allow for different bond types, right-click a bond, and select **Edit>Bond>Type.** Then select the appropriate option.
	**Bond topology –** To specify retrieval of either a ring bond or a chain bond, right-click the appropriate bond, and select **Edit>Bond>Topology.** Then select the appropriate option.
	**Position Variation Bond –** To allow specific substitution on a ring without specifying the exact site on the ring, select the atoms in the ring where substitution is allowed. Then selec**t Edit Structure>Add>Position Variation Bond.**

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