Searching for Inorganic Substances using the Molecular Formula Search Field

The following inorganic compounds can be searched within Reaxys:

- Each individual element
- All compounds without carbon
- Alloys and multi-component systems with carbon components
- Carbides, and carbideoxides
- Carbonic acids and thio- and seleno-analoges as well as their salts
- Compounds, in which carbon is present exclusively in the form of cyanide or isocyanide, e.g. HCN, HOCN, HSCN, their isoacids and salts, dicyan, polycyan, cyanamide
- Small molecules like CO, CS, CO2, CS2, COS, or phosgene.
- Substances, which contain carbon, containing at least one element shaded in green, below:



The compounds in Reaxys are available with their structures. However, only molecular structures are indexed. Compounds such as alloys, glasses, and ceramic materials have records but no structures in the database.

The best way to begin a search for inorganic compounds is through generate structure by name. If the name you type appears in the literature the exact way you type it, then the molecule will appear in the white box enabling you to begin your search. If, however, you are unsure of the spelling, or the way you write the molecular name does <u>not</u> match with what is in the database literature, this method might not work. It does not mean that there is no data on this compound; it suggests that you should try a different search method. In the following example, generate structure from name works, but the exercise deals with the molecular formula search field.





Scenario: Search for Reactions containing ruthenium bis(2,2'-bipyridine) bis(chloride) dihydrate used as a cataylst.

- Begin with the substance and properties tab highlighted
- Click on Properites (Advanced)
- Click on the [+] sign for Identification Data
- Click on the [+] sign for Substance identification
- Click on the Molecular formula field.

Properties (Form-based) Properties (Advanced)	
Check Syntax	
	SERICA POR PIELD RESET
Identification exists	^
Substance Identification	
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Preferred RN (IDE.XPR)	
CAS Registry Number (IDE.RN)	
Chemical Name (IDE.CN)	
Chemical Name Segment (IDE.CNS	5)
Linear Structure Formula (IDE.LSF)
Fragment Molecular Formula (IDE.	FMF)
Molecular Formula (IDE.MF)	is 💙
Search MF Range (IDE.MOFO)	
Charge (IDE.CHA)	
Element Counts (IDE.ELC)	

- Leave the "is" operator selected
- Click on the ellipses to open the index
- Type the molecular formula C20H16Cl2N4Ru*2H2O. Note, the order the elements are entered does NOT matter.
- Click Transfer
- The following command will appear in the white box



Click search





• A series of structures pop up in the results window

Query Results Synti	hesis Plans	History My Alerts My Settir	ngs Help Forum Info			Register	r Login 🔻					
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• Click on the gray notebook icon underneath the first substance and select "Copy structure to Query"

7 substan	ces out of 592 cit	ations						
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1		Use as Sub-s	tructure Filter					

• You will be brought back to the query window and the structure will appear in the white box.





Query	Results	Synthesis Plans	History	My Alerts	My Settings	Help	Forum	Info	
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- Click on the "Copy to Reactions Tab" Button.
- Select the starting material radio button
- Keep as Drawn selected

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• Click Search



