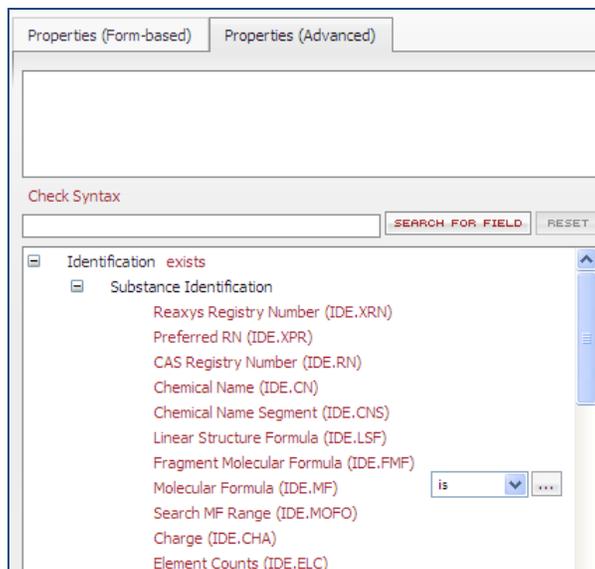




**Scenario: Search for Reactions containing** ruthenium bis(2,2'-bipyridine) bis(chloride) dihydrate **used as a catalyst.**

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



The screenshot shows the 'Properties (Advanced)' tab in the Reaxys software. Under the 'Identification exists' section, the 'Substance Identification' sub-section is expanded. A list of identification fields is shown, including Reaxys Registry Number (IDE.XRN), Preferred RN (IDE.XPR), CAS Registry Number (IDE.RN), Chemical Name (IDE.CN), Chemical Name Segment (IDE.CNS), Linear Structure Formula (IDE.LSF), Fragment Molecular Formula (IDE.FMF), Molecular Formula (IDE.MF), Search MF Range (IDE.MOFO), Charge (IDE.CHA), and Element Counts (IDE.ELC). The 'Molecular Formula (IDE.MF)' field is selected, and a dropdown menu is open showing the operator 'is'.

- Leave the “is” operator selected
- Click on the ellipses to open the index
- Type the molecular formula C<sub>20</sub>H<sub>16</sub>Cl<sub>2</sub>N<sub>4</sub>Ru\*2H<sub>2</sub>O. Note, the order the elements are entered does NOT matter.
- Click Transfer
- The following command will appear in the white box

```
IDE.MF = 'C20H16Cl2N4Ru*2H2O '
```

- Click search

- A series of structures pop up in the results window

7 substances out of 592 citations

Filter by:

- Sub-structure
- Molecular Weight
- Number of Fragments
- Physical Data
- Spectroscopic Data
- Bioactivity
- Natural Product
- Availability
- Document Type
- Authors
- Patent Assignee
- Journal Title
- Publication Year

Structure	Chemical Name	N° of preparations All Preps   All Reactions	Available Data	N° of ref.	Boiling Point
	cis-dichloro bis(2,2'-bipyridine) ruthenium(II) dihydrate bis(2,2'-bipyridine)ruthenium(II) dichloride dihydrate ruthenium bis(2,2'-bipyridine) bis(chloride) dihydrate ruthenium(II)bis(2,2'-bipyridine)dichloride dihydrate bis(2,2'-bipyridine)dichlororuthenium(II) dihydrate dichlorobis(2,2'-bipyridine)ruthenium(II) dihydrate bis(2,2'-bipyridyl)dichlororuthenium(II) dihydrate	6 prep out of 703 reactions.	Identification Physical Data (4) Spectra (8)	308	
	cis-[bis(2,2'-bipyridine)dichlororuthenium(II)] dihydrate cis-[ruthenium(II)bis(2,2'-bipyridine)dichloride] dihydrate cis-bis(2,2'-bipyridine)-ruthenium(II)dichloride dihydrate cis-[bis(2,2'-bipyridine)dichlororuthenium(II)] dihydrate cis-[dichlorobis(2,2'-bipyridine)ruthenium(II)] dihydrate cis-bis(2,2'-bipyridyl)dichlororuthenium(II) dihydrate cis-dichloro-bis(2,2'-bipyridin)ruthenium(II) dihydrate	4 prep out of 680 reactions.	Identification Physical Data (5) Spectra (4) Use/Application (1)	262	

- Click on the gray notebook icon underneath the first substance and select “Copy structure to Query”

7 substances out of 592 citations

Substances (Grid) Substances (Table) Citations

Limit to Output Hide Sort by No of References

Structure

1

Reaxys-RN: 16495942  
 MF: C<sub>20</sub>H<sub>16</sub>Cl<sub>2</sub>N<sub>4</sub>Ru\*2H<sub>2</sub>O  
 MW: 520.38  
 CAS-RN:  
 Show Details  
 Copy Structure to Clipboard  
 Copy Structure to Query  
 Use as Sub-structure Filter

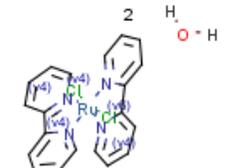
- You will be brought back to the query window and the structure will appear in the white box.

Query Results Synthesis Plans History My Alerts My Settings Help Forum Info

Reactions Substances and Properties Text, Authors and more

Generate structure from name

Double click this frame and draw structure query



As drawn

Substructure:

on heteroatoms

on all atoms

Include tautomers

Ignore stereo

No salts

No mixtures

No isotopes

No additional rings

**Further options**

COPY TO REACTIONS TAB CLEAR

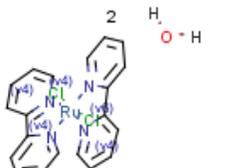
- Click on the “Copy to Reactions Tab” Button.
- Select the starting material radio button
- Keep as Drawn selected

Query Results Synthesis Plans History My Alerts My Settings Help Forum Info

Reactions Substances and Properties Text, Authors and more

Generate structure from name

Double click this frame and draw reaction query



Search as / by

Product

Starting material

Any role

Reagent/ Catalyst

As drawn

Substructure:

on heteroatoms

on all atoms

Include tautomers

Ignore stereo

No isotopes

No charges

No radicals

No additional rings

Keep Fragments separate

Ignore Atom Mappings

COPY TO SUBSTANCES TAB CLEAR

Conditions (Form-based) Conditions (Advanced)

Search

- Click Search