Reaxys Introduction Guide

This guild will explain how to search in Reaxys

1) Searching for Literature
2) Searching for Substances
3) Searching for Reactions
4) Searching for properties
5) Query Builder

1) Searching for literature

This section will show you how to search for literature in Reaxys

Start by entering your question into the text box in Reaxys

Click Find on the top right hand corner

You will be prompted by Reaxys to chose one of the options interpreted by Reaxys. You may click on Preview Results to view the top 3 hits or click on View Results to view your result set.
Reaxys utilizes natural language algorithms to interpret your search, but sometimes these algorithms may not interpret your question the way you intended. You may move your mouse over the selected option and it will review Edit in Query Builder.

Inside the Query Builder, you may see how Reaxys interpret your query and you may edit your queries as you wish.

Reaxys allows the use of truncations. You can use * as a wild card for your searches.
This search will find terms starting with Supr and Fluo.

You get hits like Fluorescence, Fluorometric, Fluorescent etc. You may use the filters at the left panel to minimize the number of hits you get.

By clicking on the substances or Reaction tab at the top, Reaxys will show you all the substances or Reactions in these 15K documents. You may also click on the substance or reaction tabs inn each bibliographic hit to view them per article.

2) Searching for Substances

This section shows you how to search for substances

You can search for substances by drawing or by text.

In this example, we will be searching for Taxol. Click on the Create Structure box
You can start drawing your structure or use one of Reaxys tools to help you draw the structure.

Click on the Create Structure template from name tab at the top right corner

You can key in the chemical name, CAS number, InChiKey or SMILES code. In this case, I typed in taxol and click on the search button

Reaxys will draw the structure for you and if you need, you may edit this structure. You may use the options on the right side to select if you are searching for as drawn, substructure or similar structures.
The other way to search the structure will be via text in the text box.

Type Taxol in the text box and do a search

Once again, Reaxys will show you the options. Select substances and click on view Results.

You may use the filters at the left to filter and select the substance you want. Notice that there are many tabs beside the substance you searched. You can sue them to find out information like Spectra, physical data (melting point, boiling point etc) Different substances will show you different tabs depending on what available data is available in Reaxys. If you click on preparation, Reaxy will show you the sysntehsis method in which the substance is the end product. If you click on Reactions, Reaxys will show you
Reactions where this substance is a part of the reaction. Documents will link you to documents showing this substance.

Sometimes after finding the substance, you may decide to purchase the. Click on the shopping cart and it will list the vendors selling them.

3) Searching for Reactions

This Section will show you how to search for Reactions in Reaxys

You may start off with the structure editor and draw your structure or use the text box.
Alternatively, you make type in the keyword “preparation” followed by the substance name.

Search Reaxys
preparation ritalin

Once again Reaxys will prompt you to select what you want. Choose Reactions.

Click on experimental procedure to expand the procedure. You may use the filters on the left to narrow down your search.
You may want to find the best synthesis route for your substances. You may click on synthesis and choose manual or auto to ask Reaxys to help you plan a synthesis route. Move your mouse over the substance. You can do this in a substance search as well.

You can choose auto or manually.
Choose the plan that suits you and you can explore the experimental procedures by clicking on the icon between the 2 substances.
4) **Searching for properties**

This Section will show you how to search for properties in Reaxys

You can search for properties in the text box if you know what properties you are searching for.

Try them

Alternatively you can search for your substance and click on the properties that you are interested in.

5) **Query Builder**

This section shows you advance searching using the Query Builder
Query builder allows you to combine Molecular formula, chemical name, structure, text to help search for complex queries easily.

For example. Search for a substance with Fe and contains the chemical name diene

Using Query builder, click on molecular formula and drag Chemical name out from the right hand side options

Search for substances. This way you can find hard to draw substances without drawing them
You can search for any properties or browse the options in the right hand panel.

In this example, I am looking for natural products. Type natural products on the search field on the top right.

In this case I am looking at substances extracted from grapefruit.

You may do any combination in query builder.