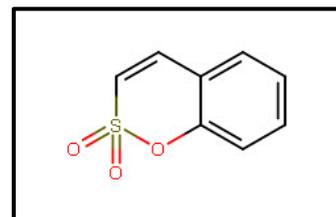


## Substance Searching

I am interested in substituted sulfocoumarins (1,2-benzoxathiine-2,2-dioxides) and would also accept results comprising of fully or partly saturated analogues. I want any substituents on carbons in the sulfur-containing ring, and I want to allow for only one substituent on the other ring.



I'd then like to quickly analyze the results to see any relationships between functional groups and various properties.

In this workflow we show examples that include:

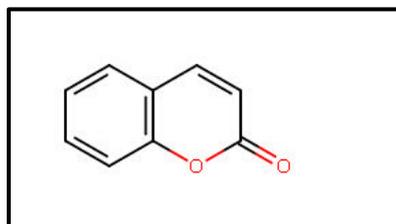
- How to create a structure template from a name
- How to make simple changes to the initial structure
- How to change the bond defaults
- How to attach a generic group at various points in the structure
- How to allow any substituent at selected points in the structure
- How to search for structures "As drawn"
- How to narrow initial answers so that they contain only those with specific functional groups

### ❖ Create a Structure Query

1. On the Reaxys home page click the **Create Structure or Reaction Drawing** box to open the structure editor (Marvin JS from ChemAxon).

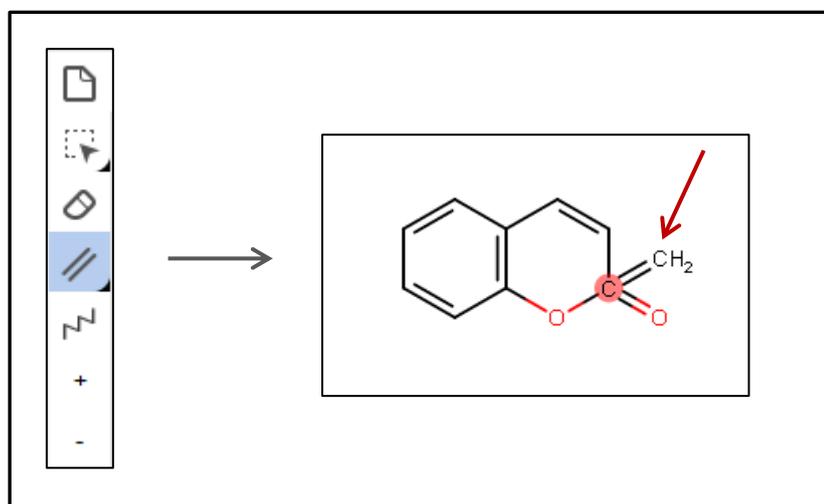


2. Draw or obtain the structure in the Marvin JS drawing panel:
  - a. Click **Create structure template from name**
  - b. Type **coumarin** and enter

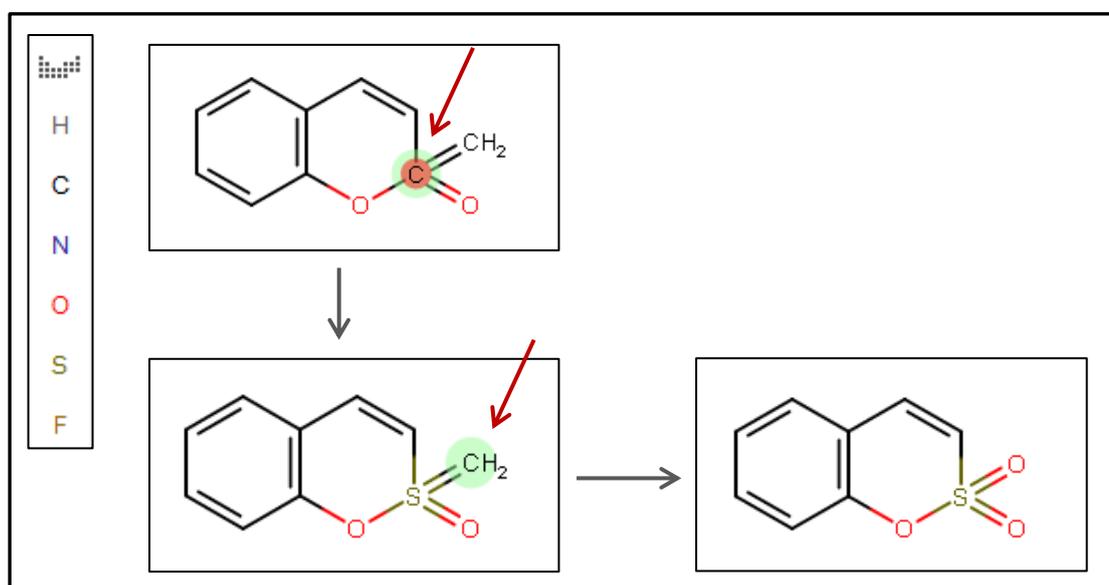


Edit the structure such that the **-O-CO-** group is replaced by **-O-SO<sub>2</sub>-**.

3. Add a double bond:
  - a. Select the **Double bond** tool
  - b. Add a bond as shown



4. Change atoms as necessary:
  - a. Click 'S' in the atom toolbar, click the 'C' atom
  - b. Click 'O' in the atom toolbar, click the 'CH<sub>2</sub>' atom



Edit the structure by adding 3 query features:

5. Add **Bond Properties**:

- Using the selection tool, select the bonds shown below (you can use the *Rectangle selection*, the *Freehand selection* (as shown below) or use the shift key to multi-select)
- Right click the selection and click **Bond properties**
- Click the **Type** drop down
- Click **any** and **Ok**

The diagram illustrates the process of adding bond properties to a chemical structure. It shows a toolbar with a selection tool, a chemical structure with a green selection box around the bonds, a context menu with 'Bond properties' selected, a 'Bond properties' dialog box with 'Type' set to 'any', and the final structure with dashed lines indicating the selected bonds.

6. Add **Position variation bond**:

- Select the bonds shown below
- Click the **Position variation bond** tool from the toolbar

The diagram illustrates the process of adding a position variation bond to a chemical structure. It shows a toolbar with the 'Position variation bond' tool selected, a chemical structure with a green selection box around the bonds, and the final structure with a methyl group (H<sub>3</sub>C) attached to the selected bonds.

7. Add the appropriate **Reaxys Generic Group (G)**:
  - a. Click the **ALK...** tool
  - b. In the **Acyclic** tab, click Any Group, in this case **G**
  - c. Click the end of the Position Variation Bond (**H<sub>3</sub>C**) to change it to **G**

8. Allow **Substituents** in 2 locations by labeling the atoms below:
  - a. Press 'Esc' on your keyboard to clear the previous tool selection
  - b. Select the two atoms shown
  - c. Right click the selection and click **Atom properties**
  - d. In the **Advanced** tab, click the **Substitutions(s)** drop down
  - e. Click **exactly** and set to **6**
  - f. Click **Ok**

The final query looks like this:

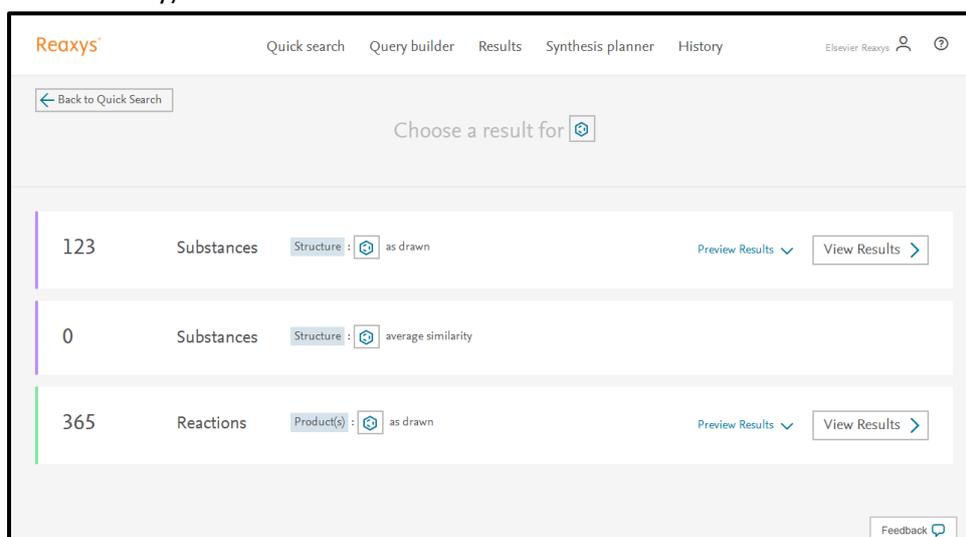
9. In the **Search this structure as:** panel, there are three options.

- **As drawn:** Reaxys will find results for the query as drawn
  - **As substructure:** Reaxys offers two sub-options:
    - **On all atoms** will substitute any explicit or implicit hydrogen with any other atom or group
    - **On heteroatoms** will do the same but only on heteroatoms
  - **Similar:** Reaxys will find results for a similarity search based on the drawn query
- a. Click **As drawn** (the query already contains substructure search features that allow for a single substituent on the C6 ring, and any substituents on the two carbons marked (s6) shown in the other ring).

10. Click **Transfer to query** and click **Search**.

The Results Preview is displayed.

- Reaxys will present a Results Preview showing 3 different variations of the entered query to provide you with options, which you may not have thought of at query formulation time:
  - Exact Substance Results for the drawn query
  - Substance Results for a similarity search based on the drawn query (*Please note: the selected substructure attributes cannot be searched for similarity, which is the reason for 0 hits*)
  - Reaction Results for the drawn query (the structure will be searched as product automatically)

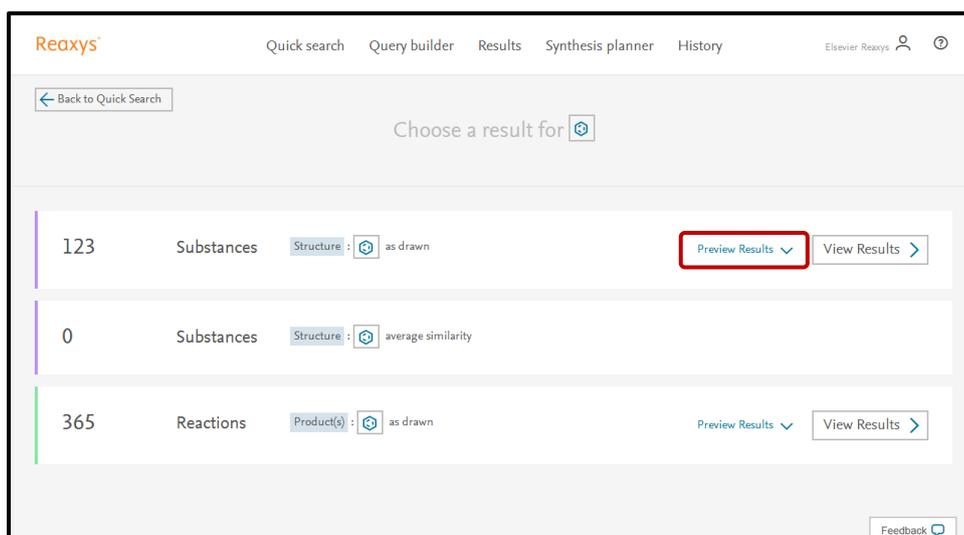


The screenshot shows the Reaxys search results preview interface. At the top, there is a navigation bar with 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. Below this is a 'Back to Quick Search' button and a 'Choose a result for' dropdown. The main content area displays three result sets:

Count	Category	Structure	Preview Results	View Results
123	Substances	Structure: as drawn	Preview Results	View Results
0	Substances	Structure: average similarity	Preview Results	View Results
365	Reactions	Product(s): as drawn	Preview Results	View Results

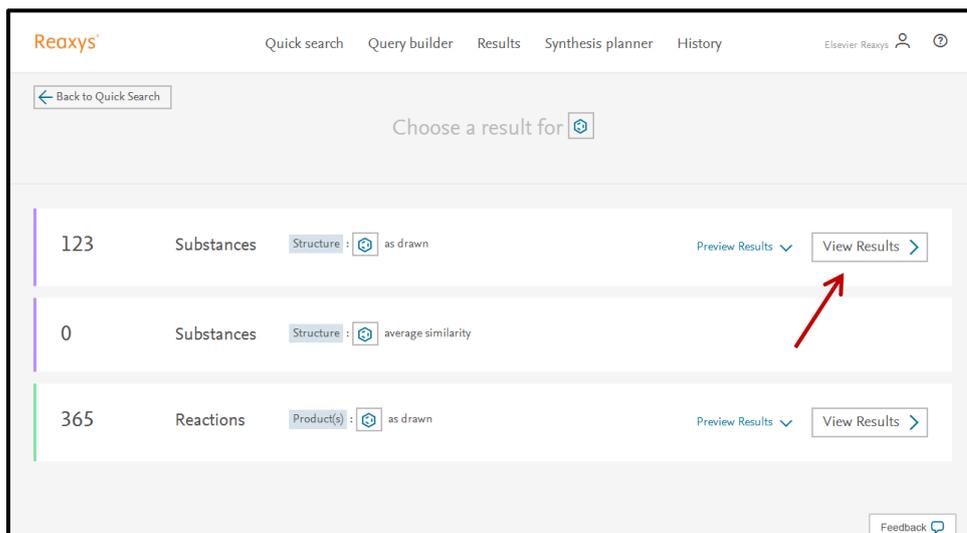
A 'Feedback' button is located at the bottom right of the interface.

- Each result set has a **Preview Results** feature that presents the top 3 results for the given query. You can check these top results before continuing to the full result set.



This screenshot is identical to the previous one, but with a red rectangular box highlighting the 'Preview Results' dropdown button for the first result set (123 Substances).

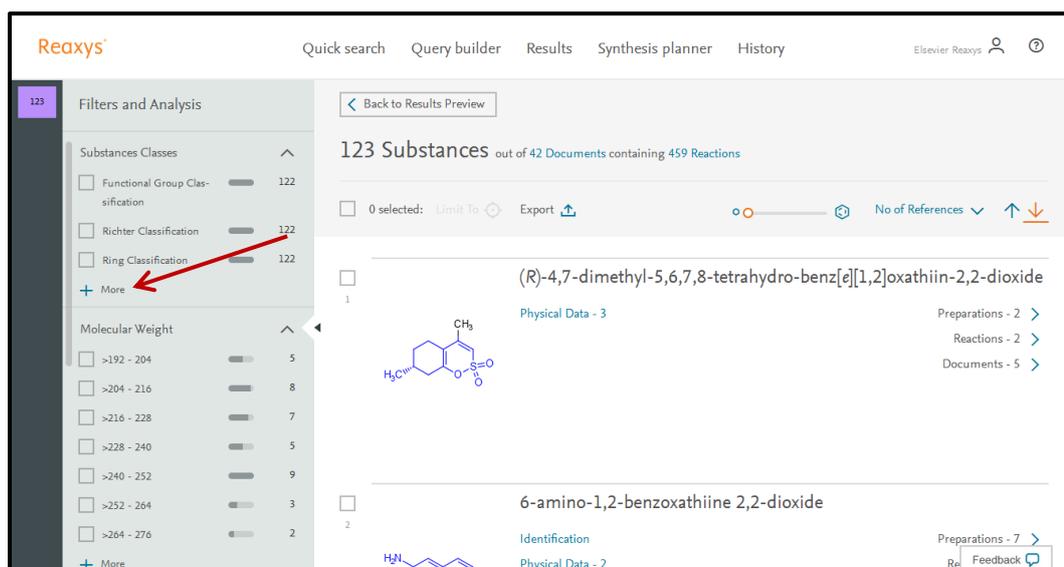
11. Click **View Results** for the first result set (Substances – as drawn).



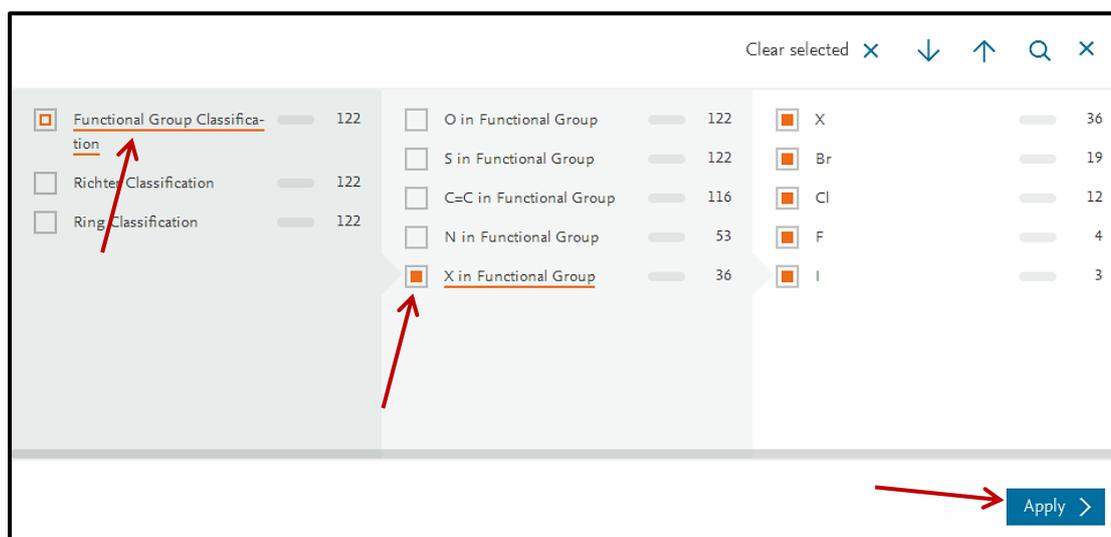
## ❖ Analyze the Results

Use the *Filter & Analysis* panel to visualize information about these compounds. For example: I want to find out when articles on compounds with certain functional groups were published for the selected Alkyl Halides.

1. Compounds are classified into structural features that can be selected from the *Substance Classes*. The list presented in the filter panel is the first level of a hierarchically organized taxonomy.
  - a. Click **+ More** to browse through the branches of the **Substance Classes** taxonomy.



- b. Click the text **Functional Group Classification**
- c. Check the box for **X in Functional Group** – to limit the results to halide compounds
- d. Click **Apply**



2. In the **Filters and Analysis** panel, collapse all filters except **Substance Classes**
  - a. Expand **Publication Year**
  - b. Check the box for **Functional Group Classification** in the Substance Classes filter.

It shows us that most of the articles about this compound have been published in the last three to four years.

The screenshot displays the search results for 36 substances. The 'Filters and Analysis' panel on the left shows the 'Substances Classes' filter expanded to 'Functional Group Classification', with 'X in Functional Group' checked. The 'Publication Year' filter is also expanded, showing counts for 2011 (13), 2013 (5), and 2015 (4). The main results area shows the first two substances: 6-bromo-1,2-benzoxathiine 2,2-dioxide and 6-iodo-1,2-benzoxathiine 2,2-dioxide, each with associated data like Preparations, Reactions, Spectra, and Documents.

*Please note:* if you select an item in one filter then items in other filters will adapt accordingly (the number displayed represents the number of substances you will get, if you apply the filter selection).