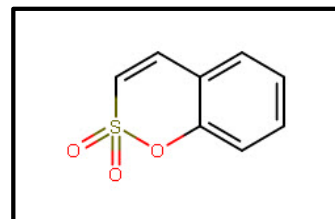


Substance Searching

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:

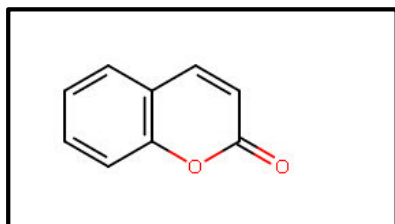
- How to create a structure template from a name
- How to make simple changes to the initial structure
- How to change the bond defaults
- How to attach a generic group at various points in the structure
- How to allow any substituent at selected points in the structure
- How to search for structures "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).

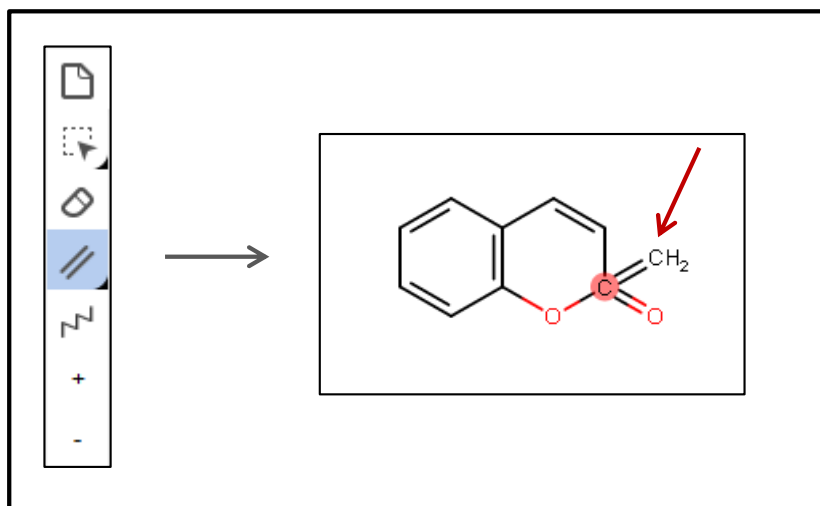


2. Draw or obtain the structure in the Marvin JS drawing panel:
 - a. Click **Create structure template from name**
 - b. Type **coumarin** and enter

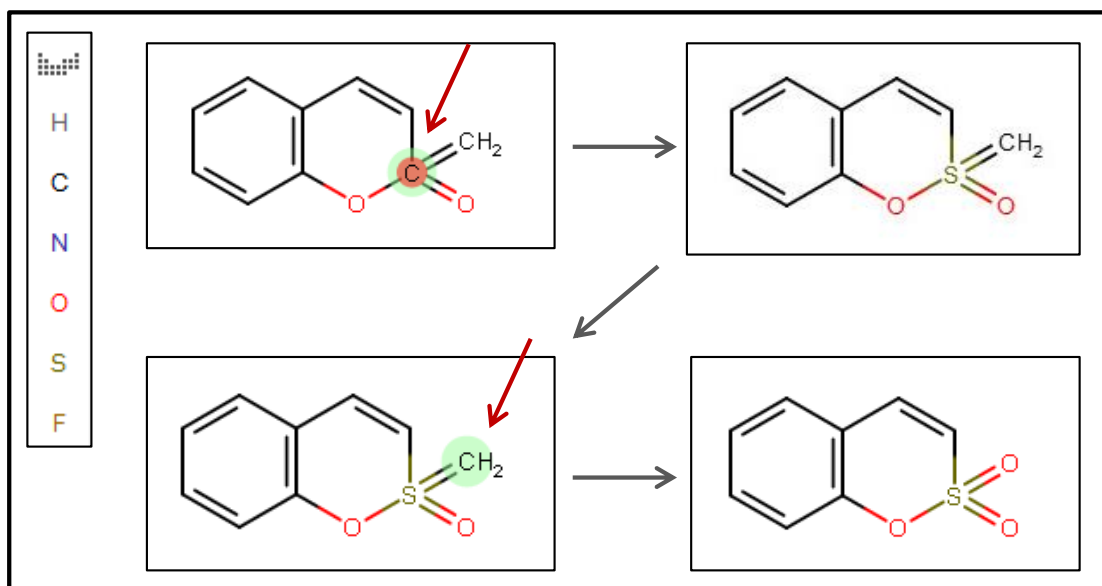


Edit the structure such that the **-O-CO-** group is replaced by **-O-SO₂-**.

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 'CH₂' 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 on the left, a chemical structure with a green freehand selection around the benzene ring and sulfur-containing group, 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 on the right, a chemical structure with a green freehand selection around the benzene ring and sulfur-containing group, and the final structure with a methyl group (H₃C) attached to the benzene ring.

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 (**H₃C**) 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).
 - b. In this example we are searching for the exact structure, therefore turn off all **Include** features

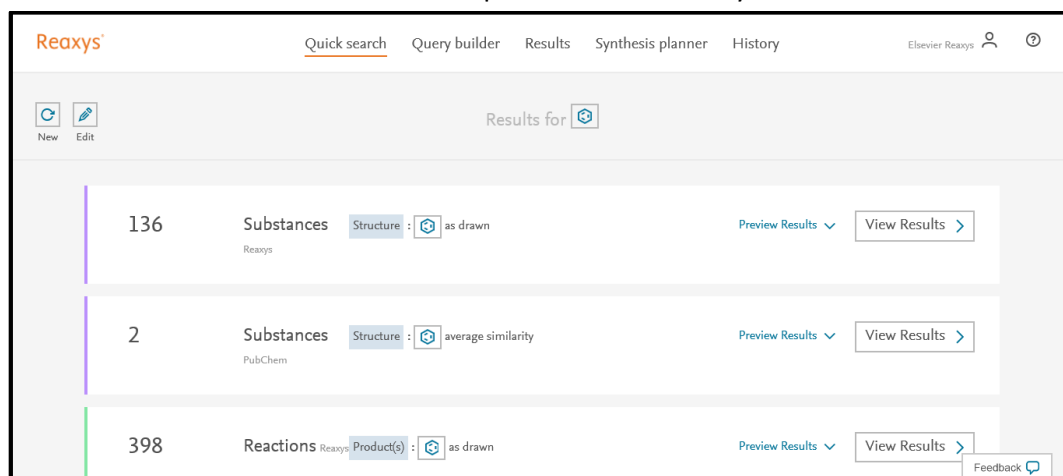
10. Click **Transfer to query** and click **Find**.

The Results Preview is displayed.

- Reaxys will present a Results Preview showing three 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
- Reaction Results for the drawn query

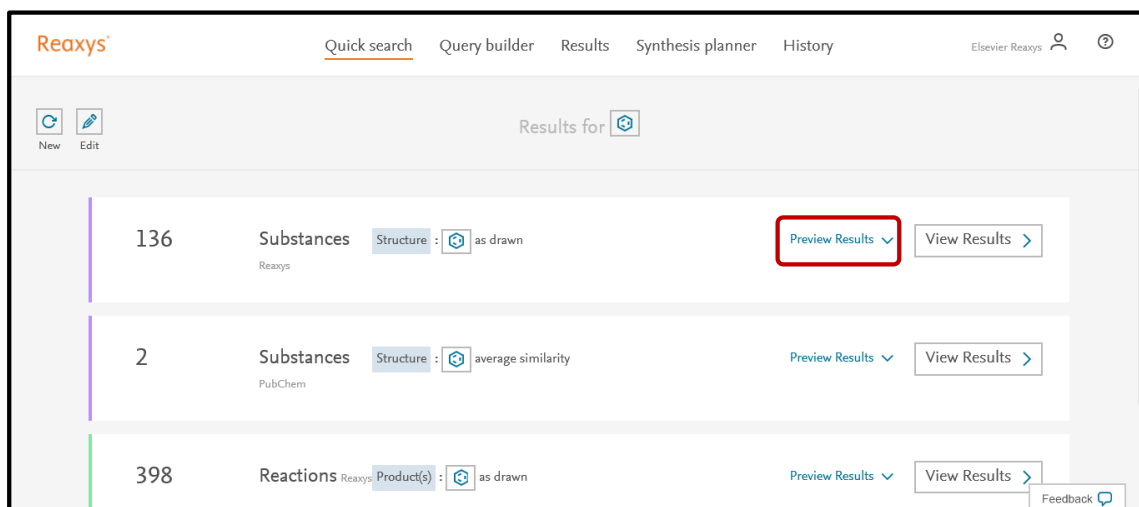
Note: the structure will be searched as product automatically



The screenshot shows the Reaxys search results interface. At the top, there are navigation tabs: Quick search, Query builder, Results, Synthesis planner, and History. The user is logged in as Elsevier Reaxys. The main content area displays 'Results for' followed by a chemical structure icon. Below this, there are three result categories, each with a count, a title, a search criteria dropdown, and two buttons: 'Preview Results' and 'View Results'.

Count	Category	Search Criteria	Preview Results	View Results
136	Substances (Reaxys)	Structure: as drawn	Preview Results	View Results
2	Substances (PubChem)	Structure: average similarity	Preview Results	View Results
398	Reactions (Reaxys)	Product(s): as drawn	Preview Results	View Results

- Each result set has a **Preview Results** feature that presents the top three 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 the 'Preview Results' button for the first category (136 Substances) is highlighted with a red rectangular box to draw attention to it.

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. Expand *Substances Classes*

- b. Click **+ More** to browse through the branches of the **Substance Classes** taxonomy.

Reaxys® Quick search Query builder Results Synthesis planner History Elsevier Reaxys

136 Filters and Analysis

136 Substances out of 44 Documents containing 492 Reactions

By Structure

Substances Classes

- Functional Group Classification 135
- Richter Classification 135
- Ring Classification 135
- + More**
- Molecular Weight
- Availability
- Available Data
- Document Type

1 (R)-4,7-dimethyl-5,6,7,8-tetrahydro-benz[e][1,2]oxathiin-2,2-dioxide
C₁₂H₁₄O₂S 214.285 7928 63549-11-1

Physical Data - 3 Preparations - 2 >
Reactions - 2 >
Documents - 5 >

2 6-amino-1,2-benzoxathiin 2,2-dioxide
C₈H₇NO₂S 197.214 22787284 1383813-19-1

Identification Preparations - 7 >
Physical Data - 2 Reactions - 51 >
Spectra - 4

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

Substances Classes

- Functional Group Classification** 135
 - Richter Classification 135
 - Ring Classification 135
 - O in Functional Group 135
 - S in Functional Group 135
 - C=C in Functional Group 129
 - N in Functional Group 54
 - X in Functional Group** 44
 - C#C in Functional Group 1
- X 44
- Br 20
- Cl 13
- F 10
- I 3

Apply >

- In the **Filters and Analysis** panel, check the box for **Functional Group Classification** in the Substance Classes filter.

The screenshot shows the Reaxys interface with the 'Filters and Analysis' panel on the left. Under 'Substances Classes', the 'Functional Group Classification' checkbox is checked, and a red arrow points to it. The main results area shows 44 substances. Two examples are visible: 6-bromo-1,2-benzoxathiine 2,2-dioxide (C₈H₇BrO₃S, 261.096, 13412914) and 6-iodo-1,2-benzoxathiine 2,2-dioxide (C₈H₇IO₃S, 308.096, 26685950, 1571901-96-6). Each entry includes a chemical structure, identification, physical data, spectra, and bioactivity links.

- Scroll down and expand **Publication Year**

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

This screenshot shows the same search results as the previous one, but with the 'Publication Year' filter expanded in the 'Filters and Analysis' panel. A red box highlights the years 2011 (13 substances), 2016 (8 substances), 2013 (5 substances), and 2015 (4 substances). The rest of the interface remains the same.

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).