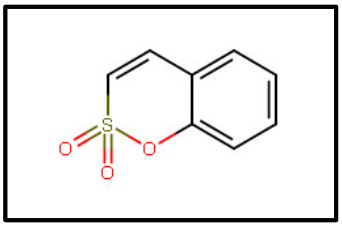
Substance Searching



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.

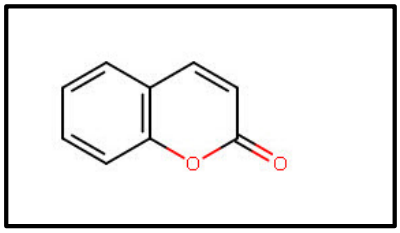
In this workflow we show examples that include:

- 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

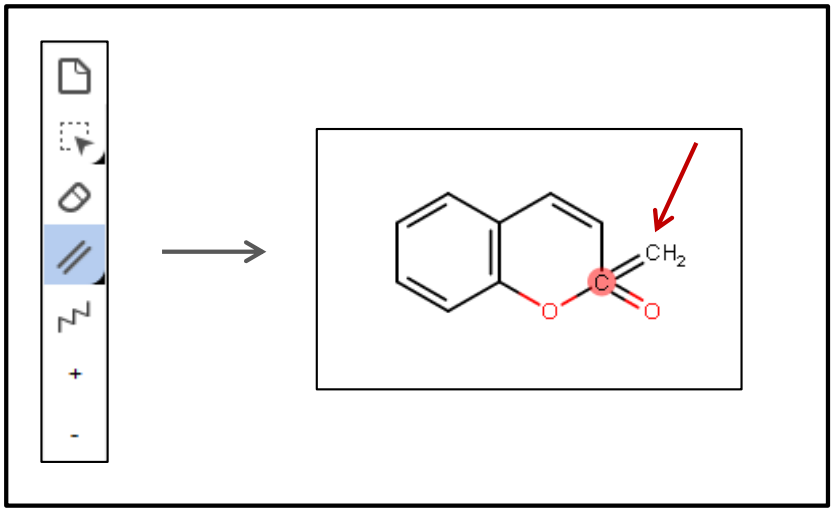
1. On the Reaxys home page click the ***Create Structure or Reaction Drawing*** box to open the structure editor (Marvin JS from ChemAxon).

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

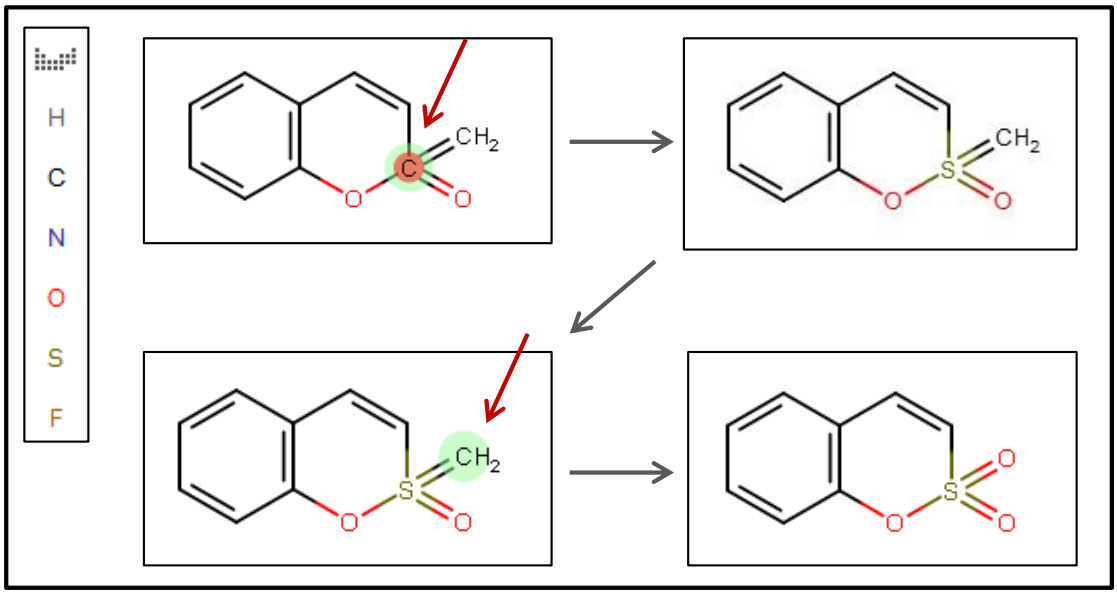


Edit the structure such that the ***–O-CO-*** group is replaced by ***–O-SO2-***.

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

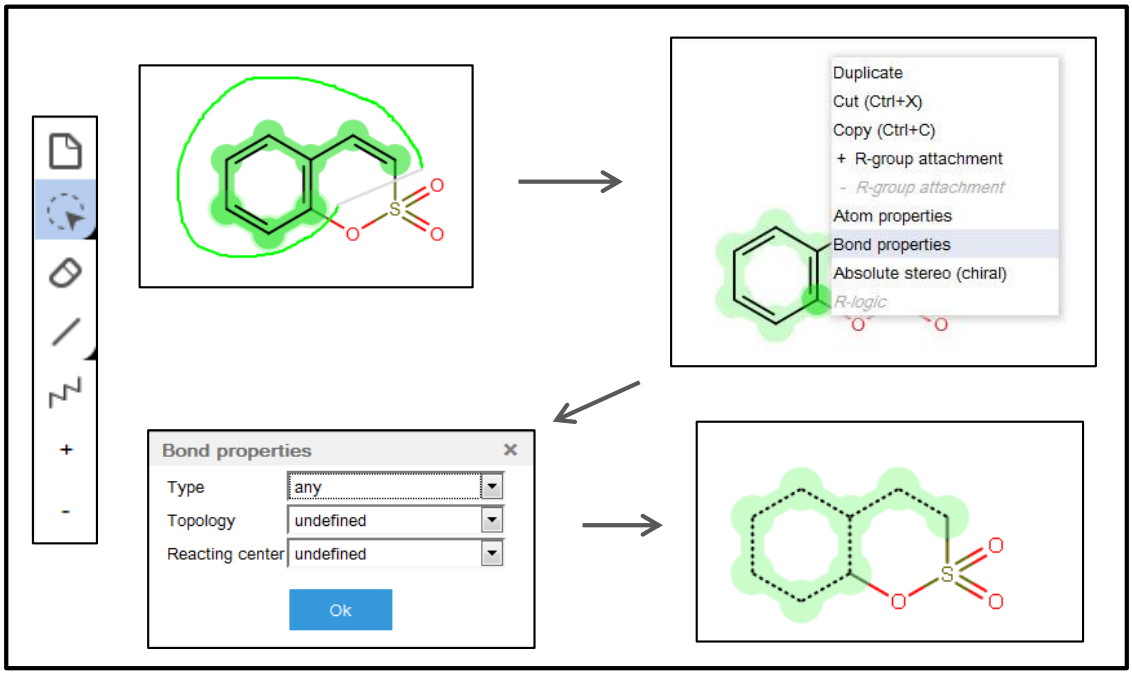


4. Change atoms as necessary:
   a. Click '***S***' in the atom toolbar, click the '***C***' atom
   b. Click '***O***' in the atom toolbar, click the '***CH_2***' atom

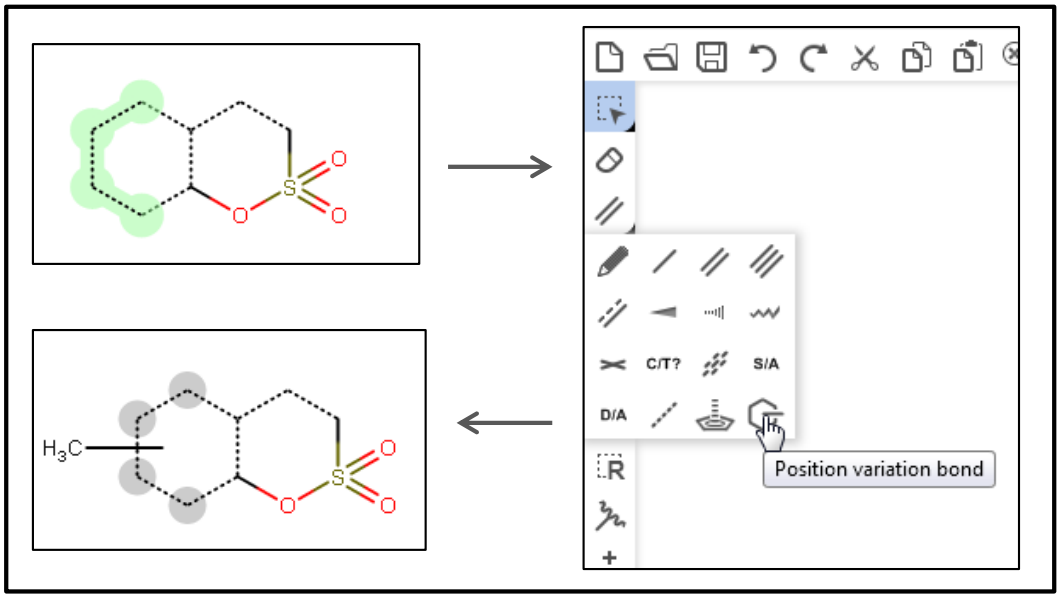


Edit the structure by adding 3 query features:

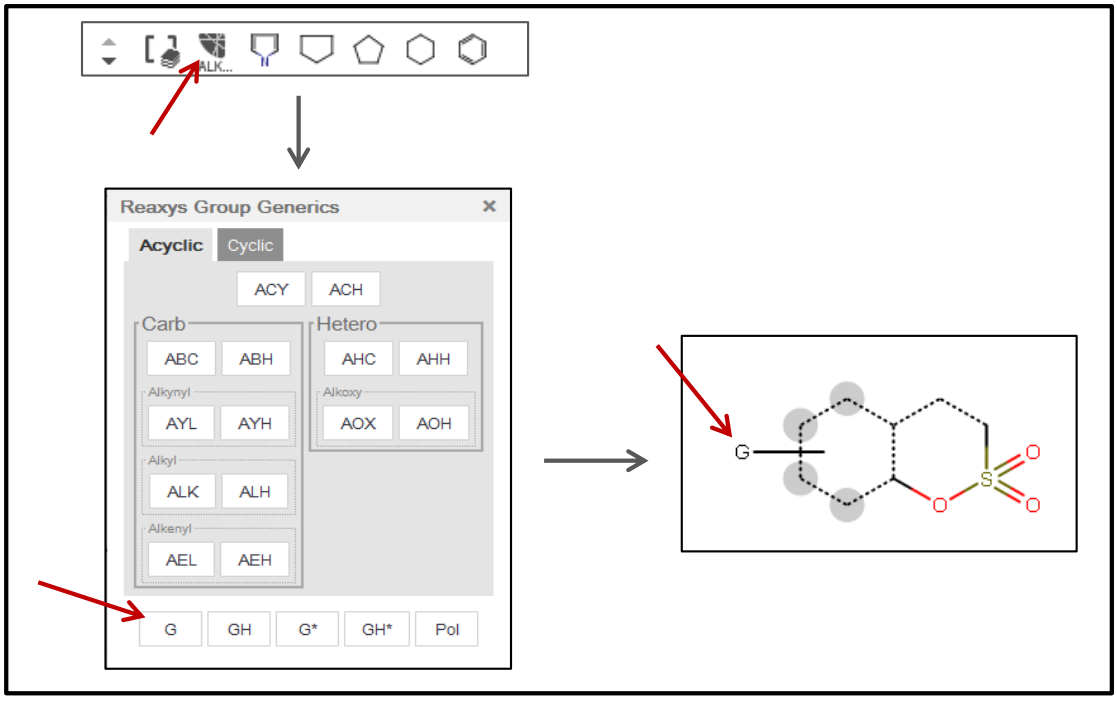
5. Add **Bond Properties**:
   a. Using the selection tool, select the bonds shown below (you can use the *Rectangle selection*, the ***Freehand selection*** (as shown below) or use the shift key to multi-select)
   b. Right click the selection and click ***Bond properties***
   c. Click the ***Type*** drop down
   d. Click ***any*** and ***Ok***



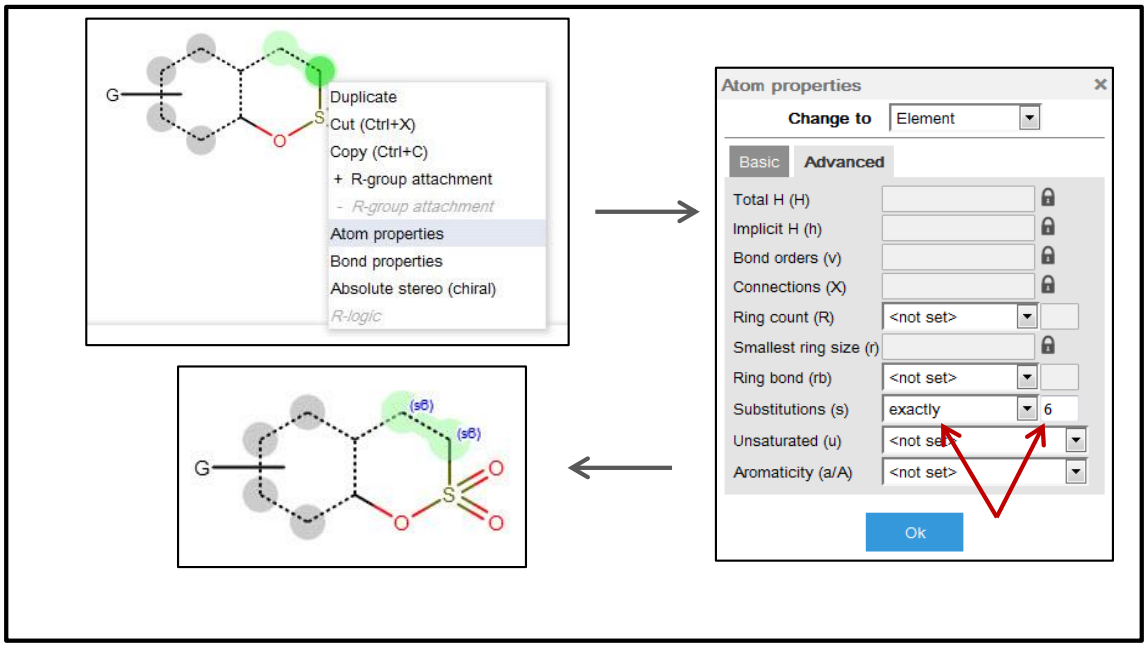
6. Add **Position variation bond**:
   a. Select the bonds shown below
   b. Click the ***Position variation bond*** tool from the toolbar



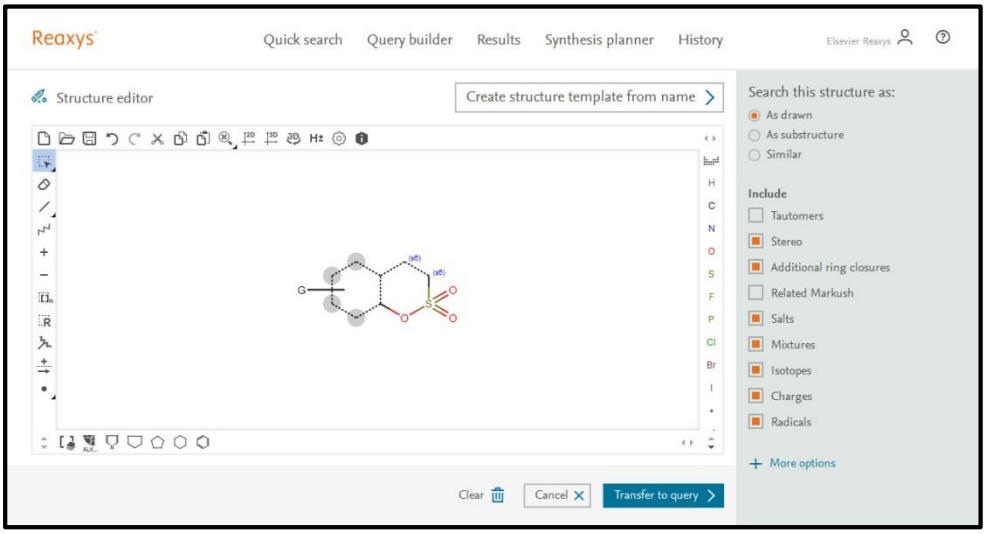
7. Add the appropriate **Reaxys Generic Group (G)**:
   a. Click the ***ALK…*** tool
   b. In the ***Acyclic*** tab, click Any Group, in this case ***G***
   c. Click the end of the Position Variation Bond (***H_3C***) to change it to ***G***



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***

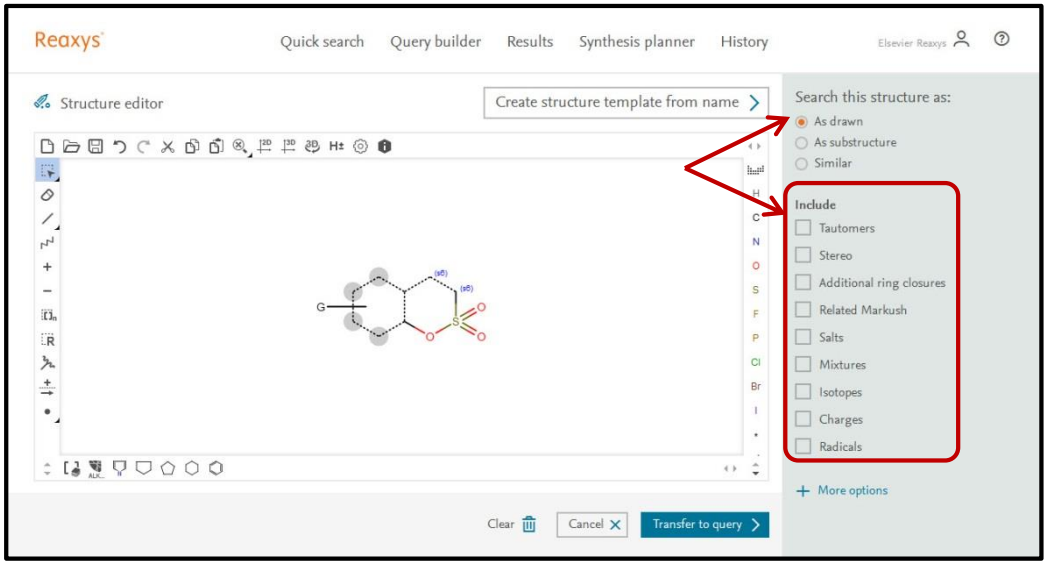


The final query looks like this:

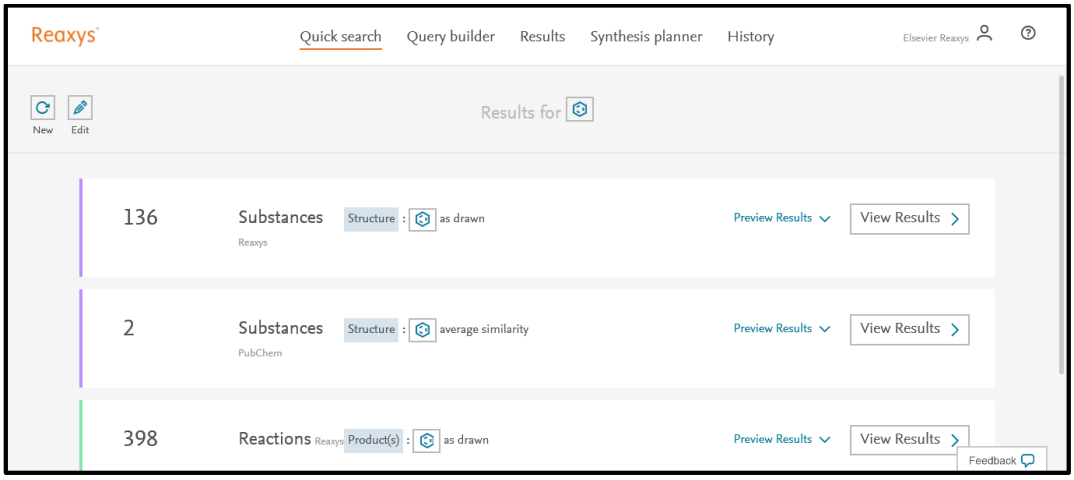


9. In the **Search this structure as**: panel, there are three options.
    - **As drawn**: Reaxys will find results for the query as drawn
    - **As substructure**: Reaxys offers two sub-options:
        - **On all atoms** will substitute any explicit or implicit hydrogen with any other atom or group
        - **On heteroatoms** will do the same but only on heteroatoms
    - **Similar***:* Reaxys will find results for a similarity search based on the drawn query

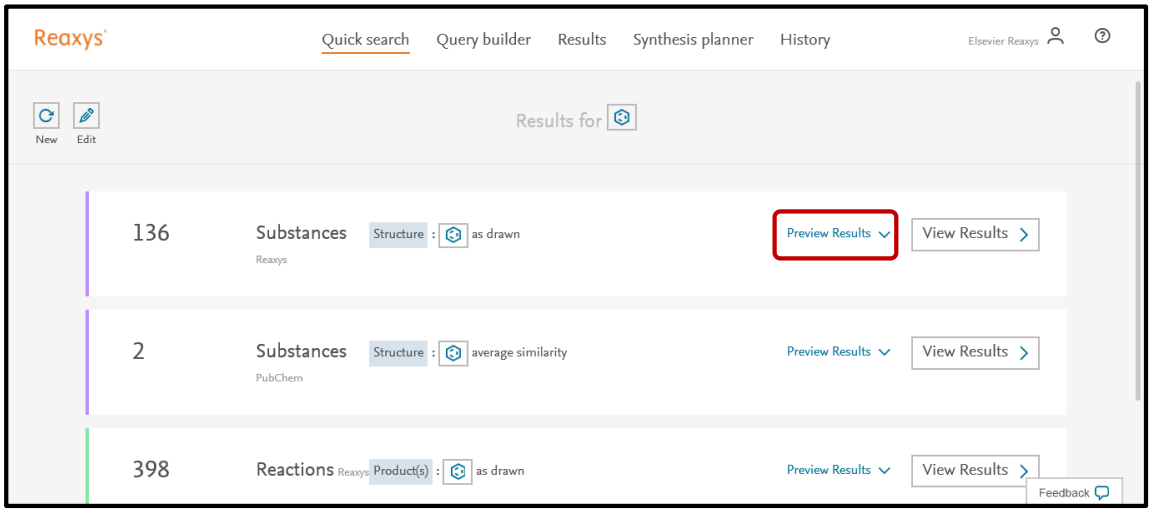
    a. Click ***As drawn*** (the query already contains substructure search features that allow for a single substituent on the C6 ring, and any substituents on the two carbons marked (s6) shown in the other ring).
    b. In this example we are searching for the exact structure, therefore turn off all ***Include*** features



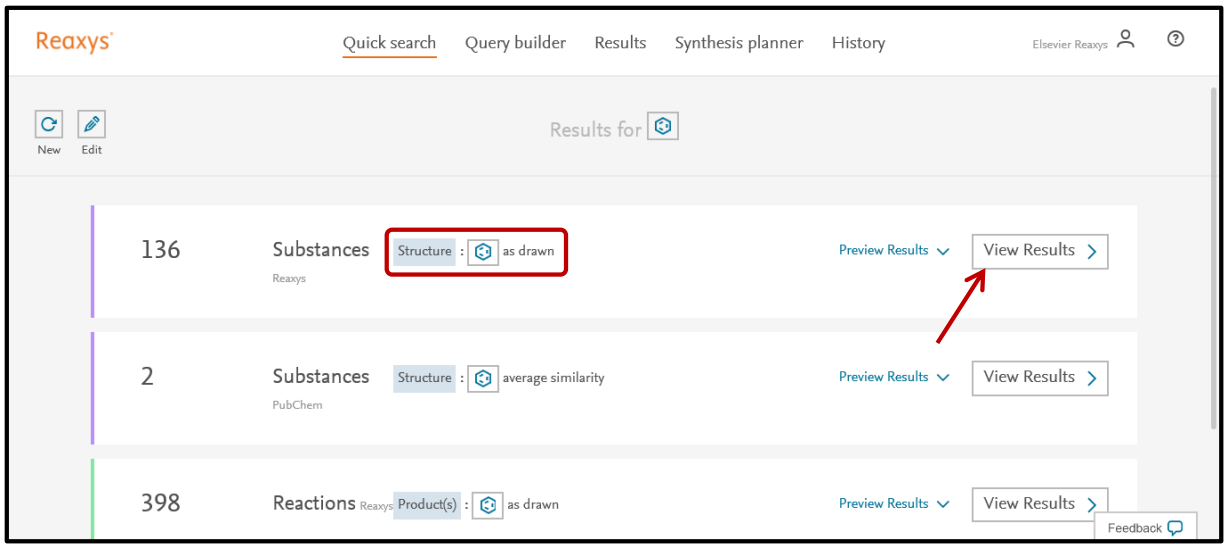
10. Click ***Transfer to query*** and click ***Find***.
    The Results Preview is displayed.
    - Reaxys will present a Results Preview showing three different variations of the entered query to provide you with options, which you may not have thought of at query formulation time:
        - Exact Substance 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



- 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.



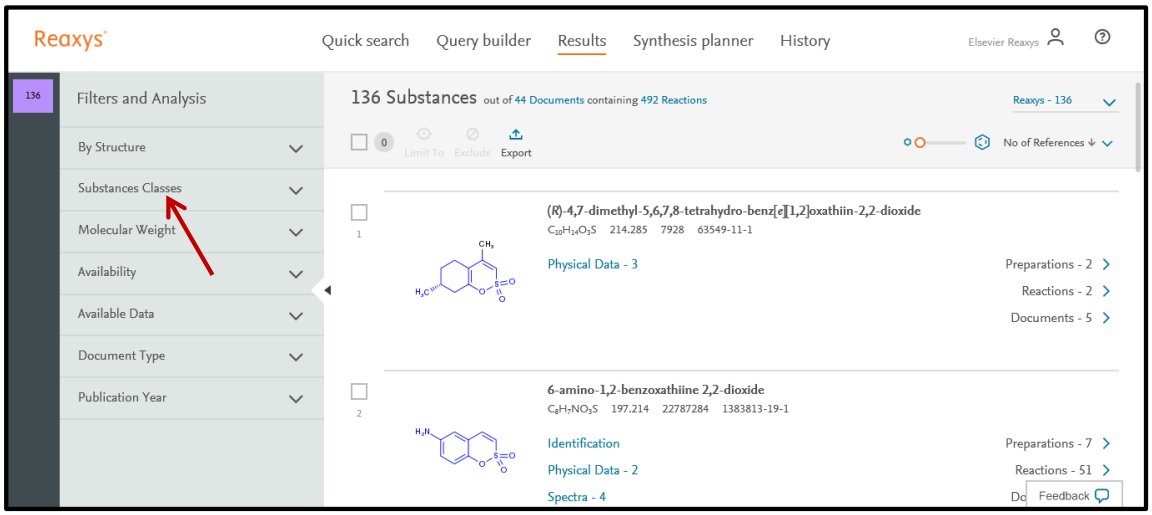
11. Click ***View Results*** for the first result set (Substances – as drawn).



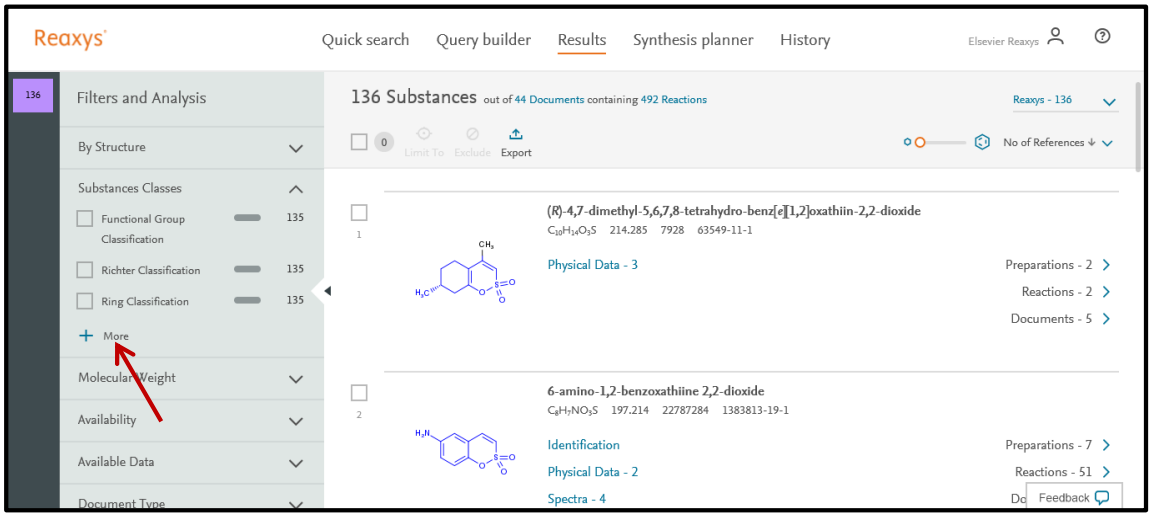
❖ Analyze the Results

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***



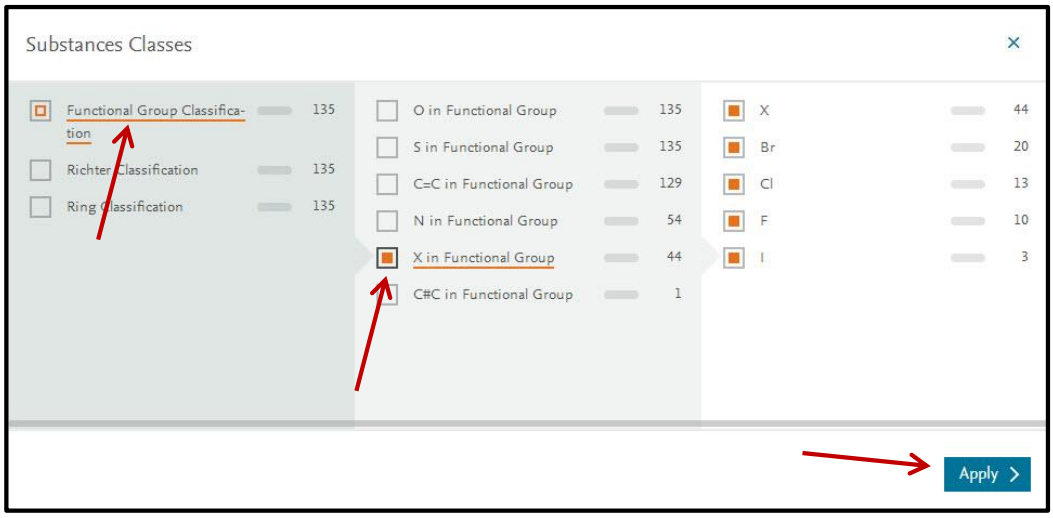
b. Click ***+ More*** to browse through the branches of the ***Substance Classes*** taxonomy.



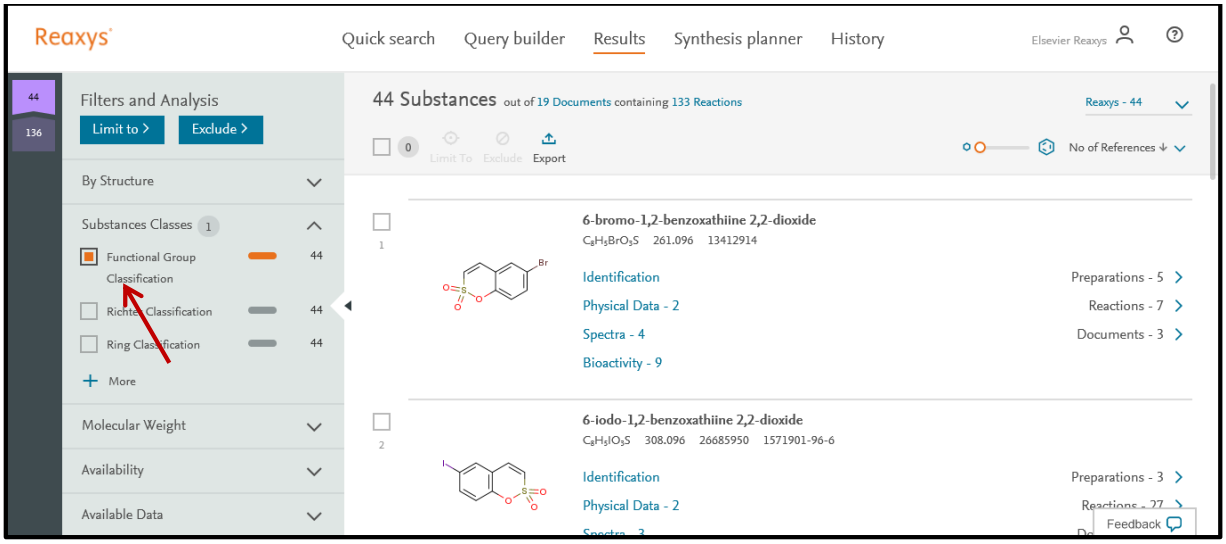
c. Click the text ***Functional Group Classification***

d. Check the box for ***X in Functional Group*** – to limit the results to halide compounds

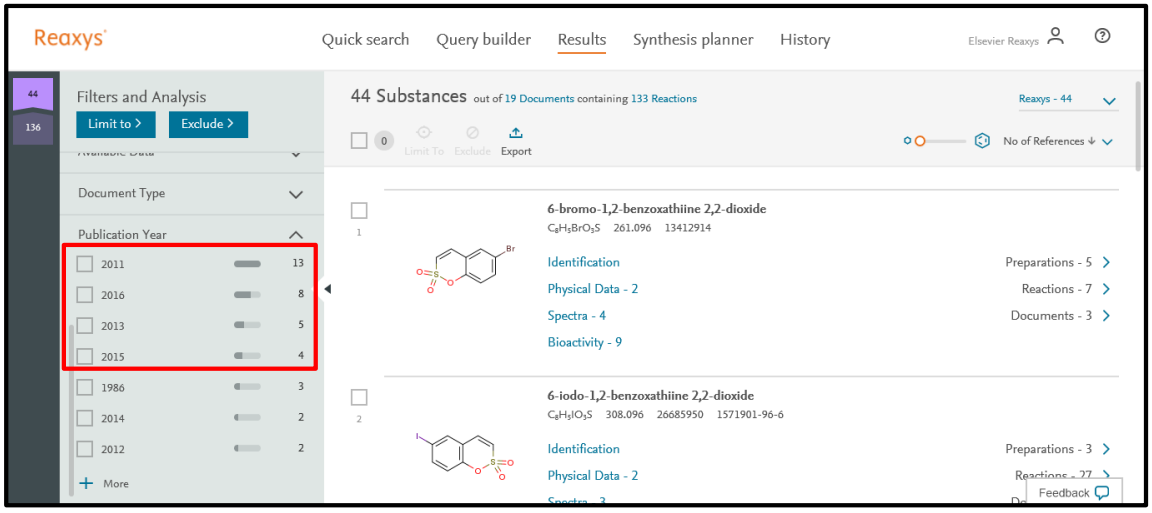
e. Click ***Apply***



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



a. 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.



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).