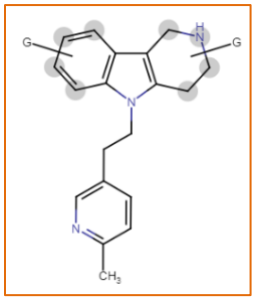
Reaxys®

Workflow example

Exploring synthetic strategies for the synthesis of dimebon analogs

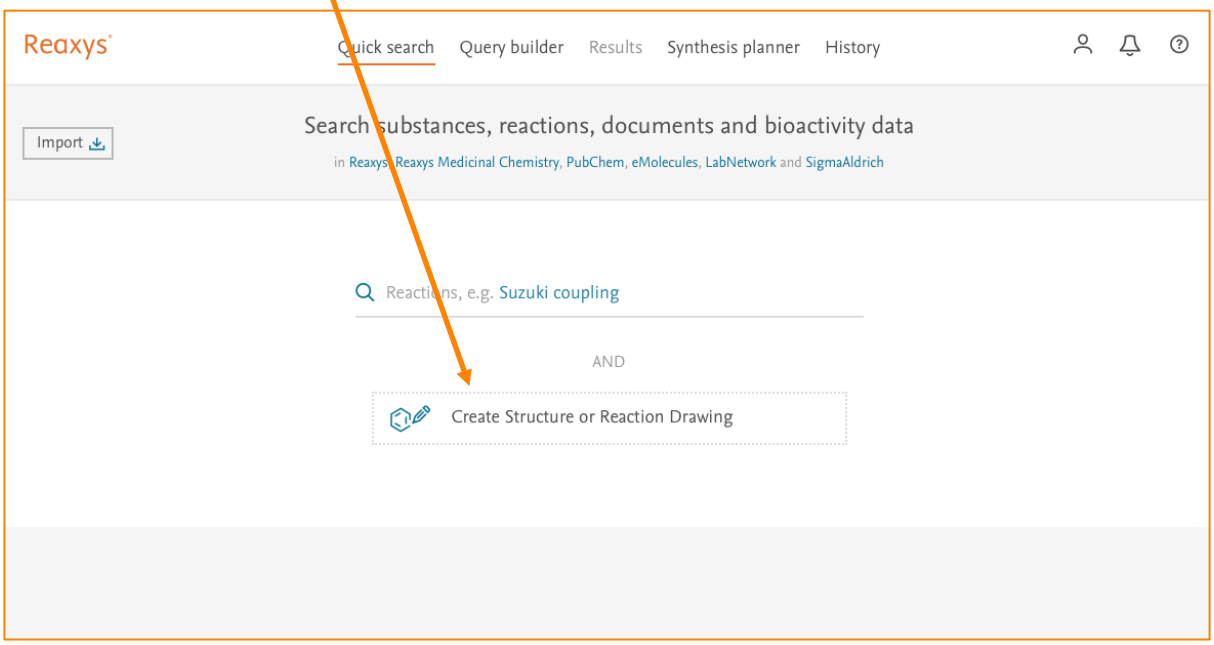
Workflow concept

Using Reaxys, the scientist wishes to explore the different synthetic strategies available for the synthesis of analogs of the antihistamine dimebon, which has the following structure.

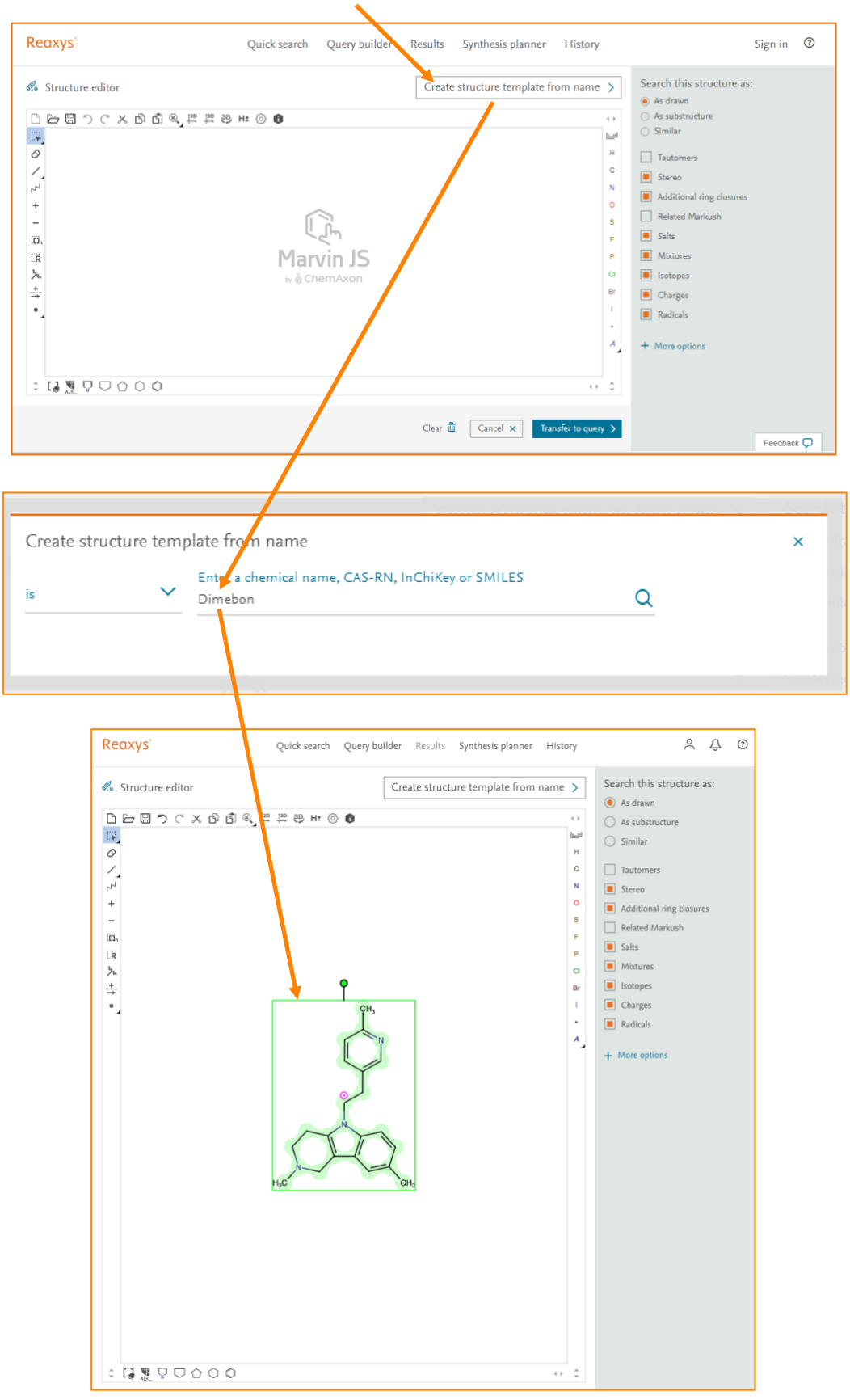


1. Use the drawing tool in Quick Search to create the desired structure

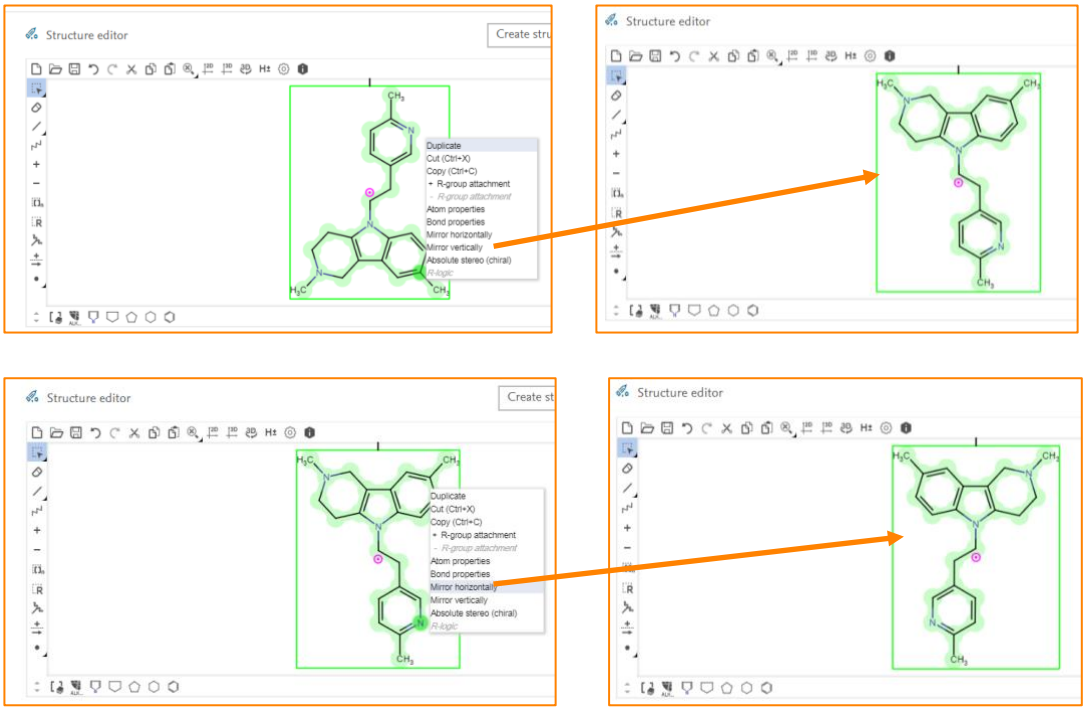
Click on **Create Structure or Reaction Drawing** in Quick Search.



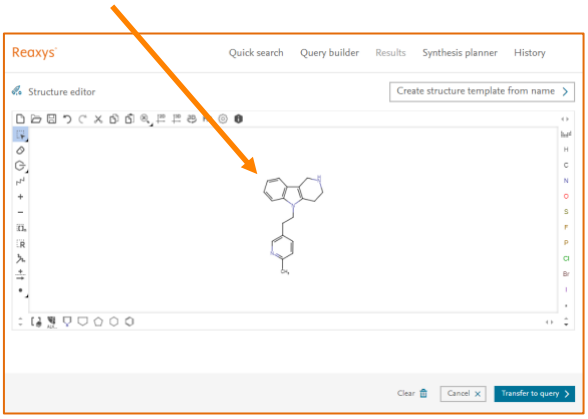
Click **Create structure template from name** and type “Dimebon”. The structure will autopopulate.



To change the orientation of the structure, right click on any atom and select **Mirror Vertically** or **Mirror Horizontally**.

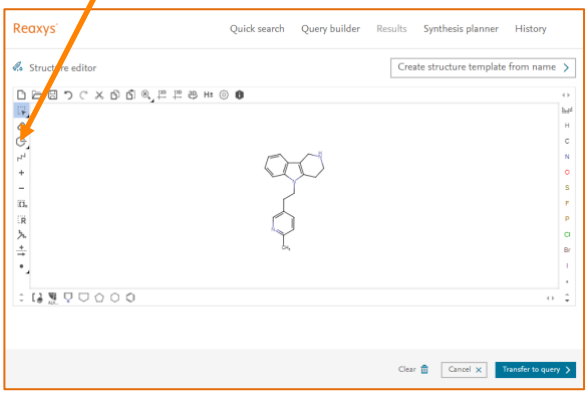


You can adjust the size of the structure by scrolling up or down. Remove the two methyl groups from the upper rings by clicking on the C and hitting Delete on your keyboard.

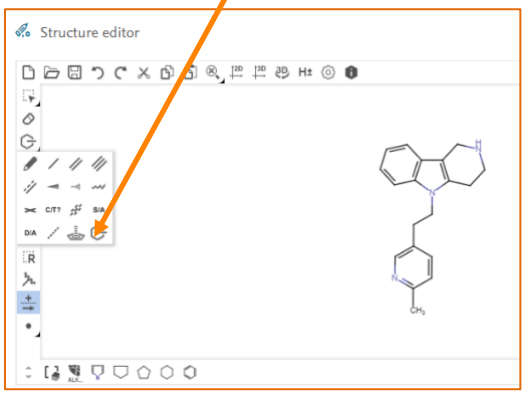


Place position variation bonds as follows:

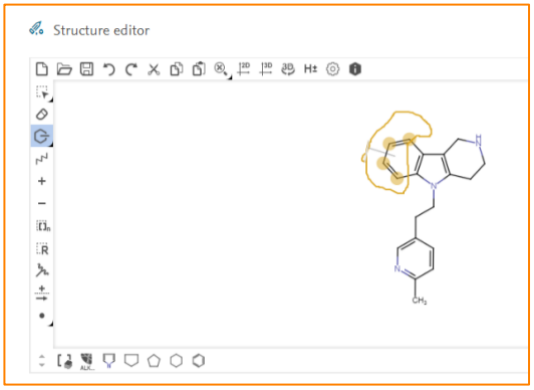
a. Click here to open the tool panel.

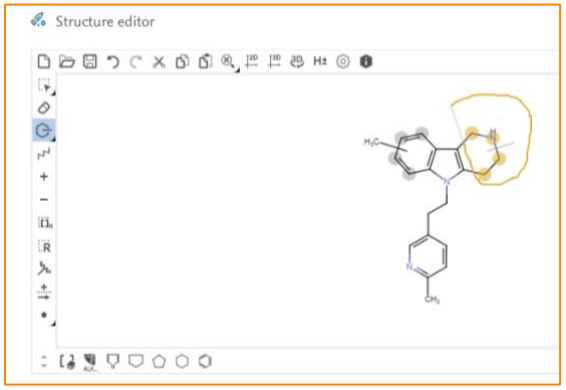


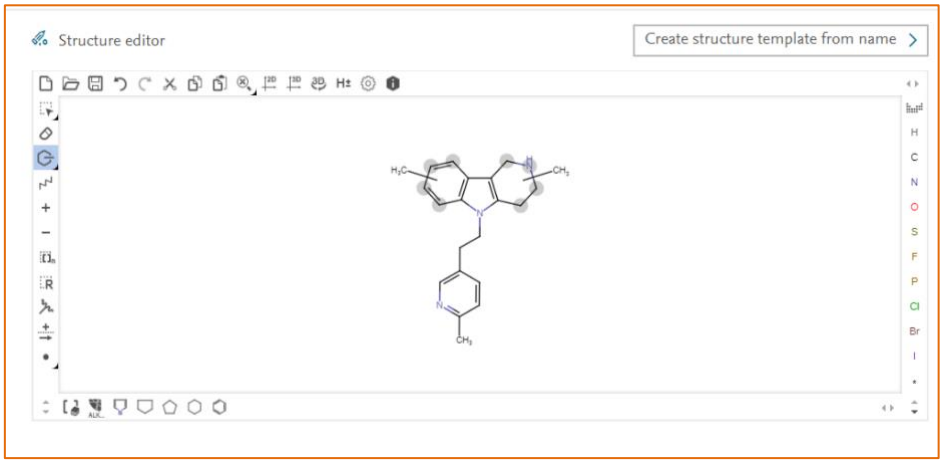
b. Select the position variation bond.



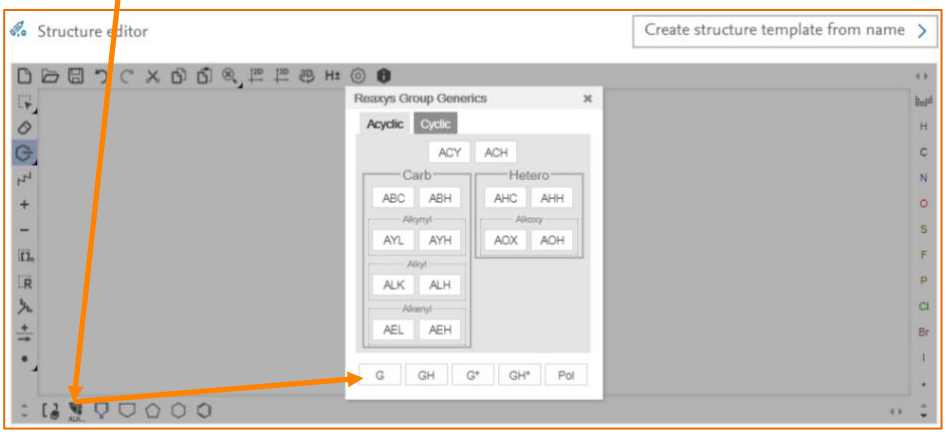
c. Select the atoms to be included by drawing a line around them.





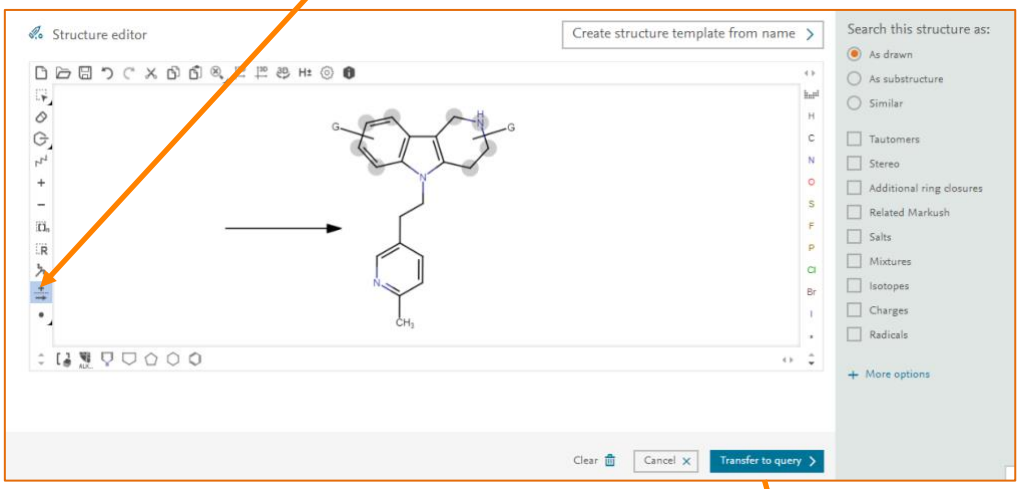


Open the **Group Generics** dialog box with the button in the bottom panel. Select **G**.

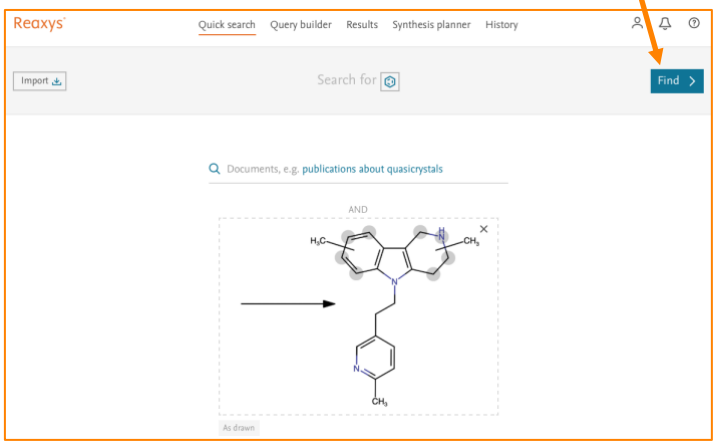


This allows the addition of any group as a query at the position variation bond.

Add the reaction arrow from the left panel to ensure that the query structure is searched as a product.

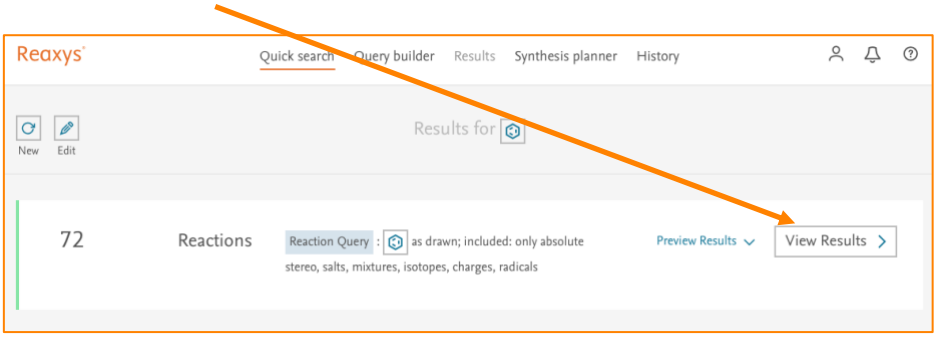


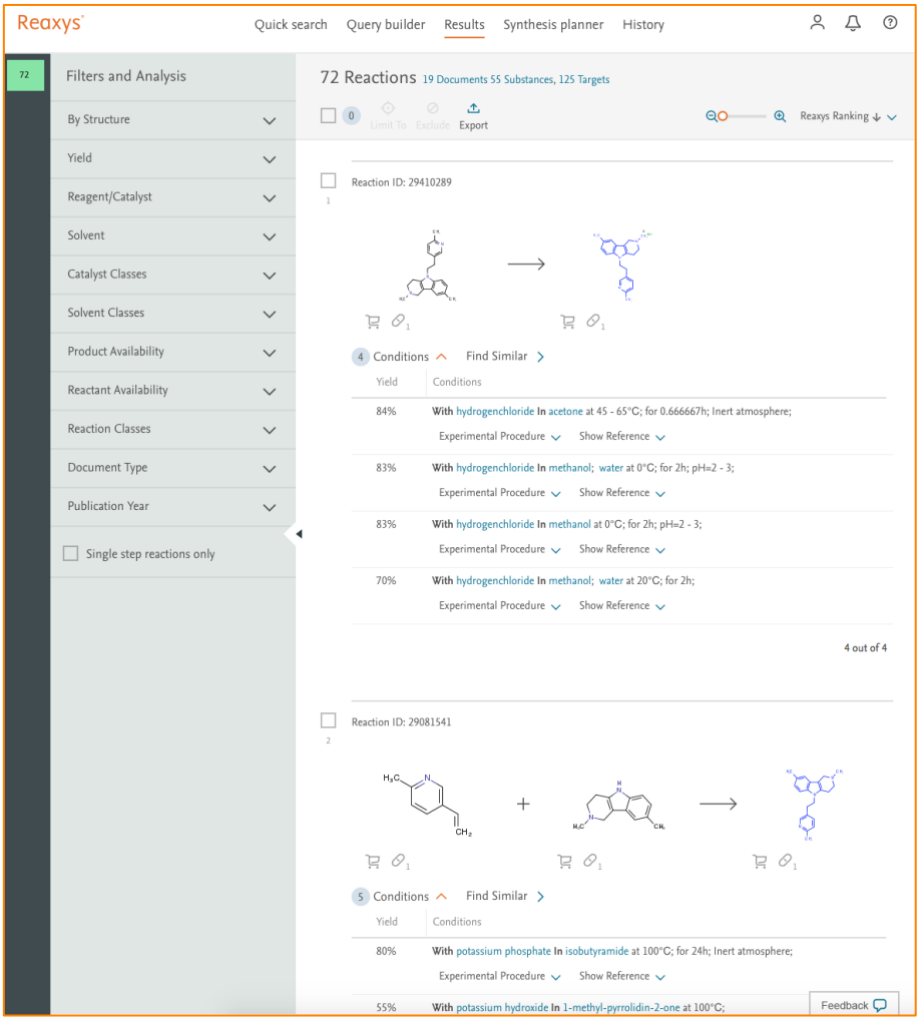
Click **Transfer to query** and then **Find**.



2. View results

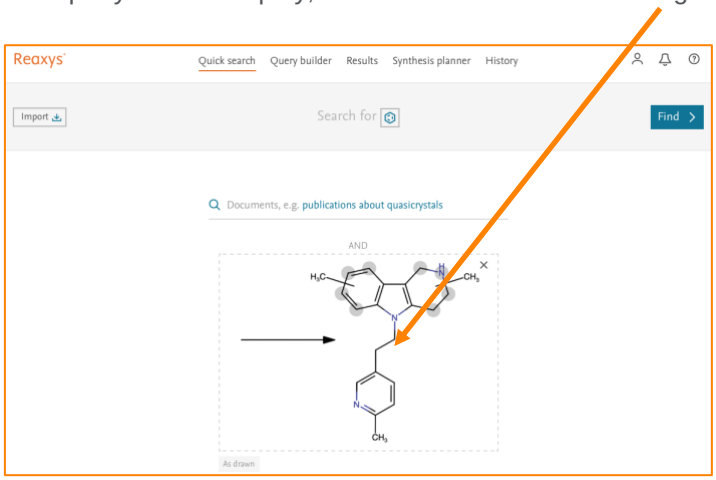
In this search, Reaxys finds 72 reactions with the dimebon structure with position variation bonds as a product. Click on **View Results** to explore the details of the reactions.



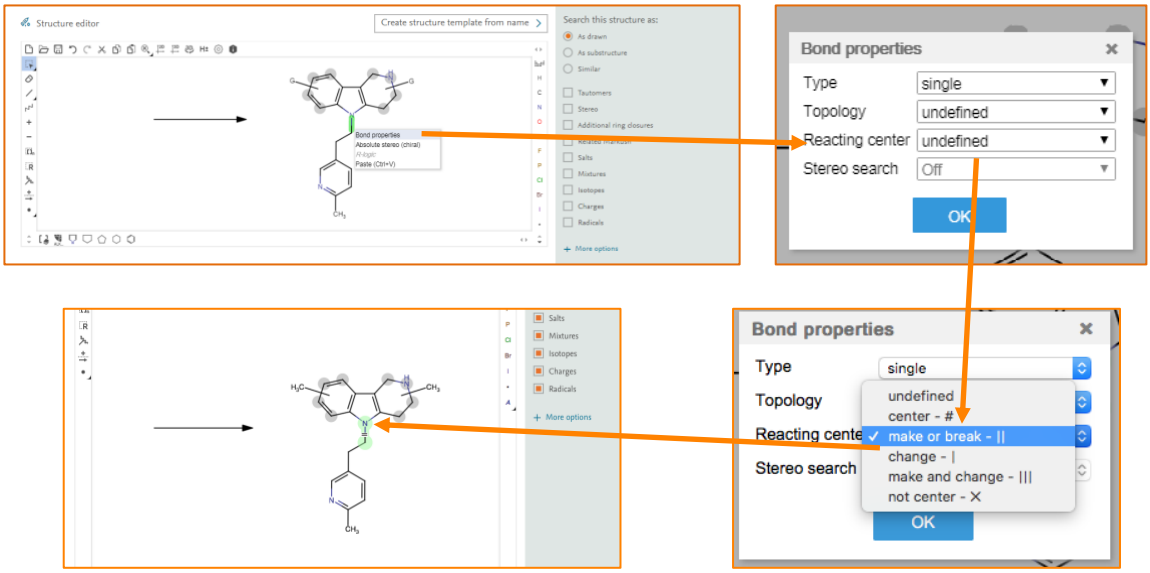


3. Explore reactions around specific bonds

Click **Quick Search**. The query will still display, as before. Click on the drawing to re-open the editor.

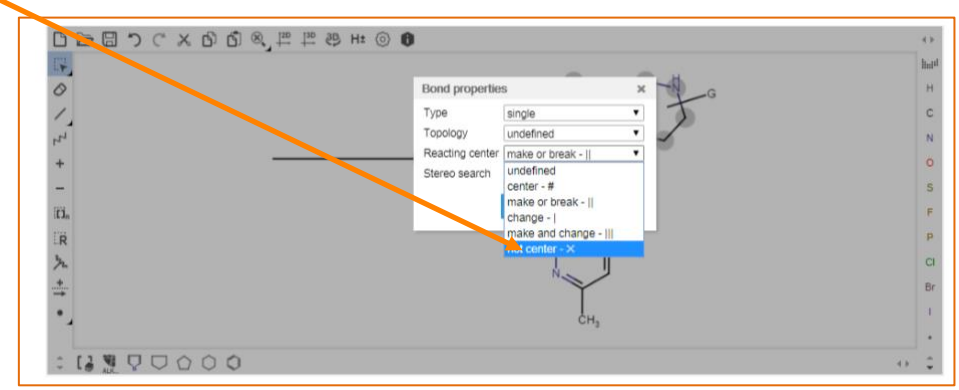


Right click on the bond and click Bond properties. Click the dropdown menu for **Recting center** and define it as **make or break**. This will enable a search of those reactions where this bond is either making or breaking. As before, transfer this to your query and click **Find**.



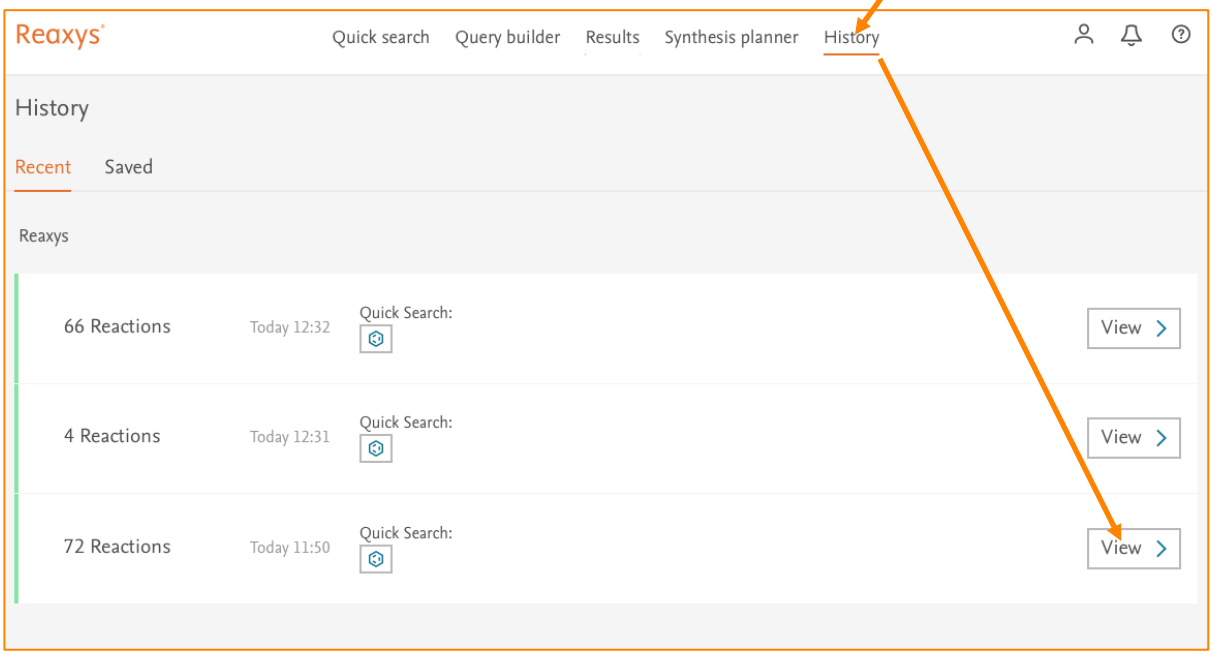
The relevant reactions can be explored in more detail in the results.

To search for reactions where the bond is not involved, open the query structure and select **Not center** from the **Reacting center** dropdown menu.

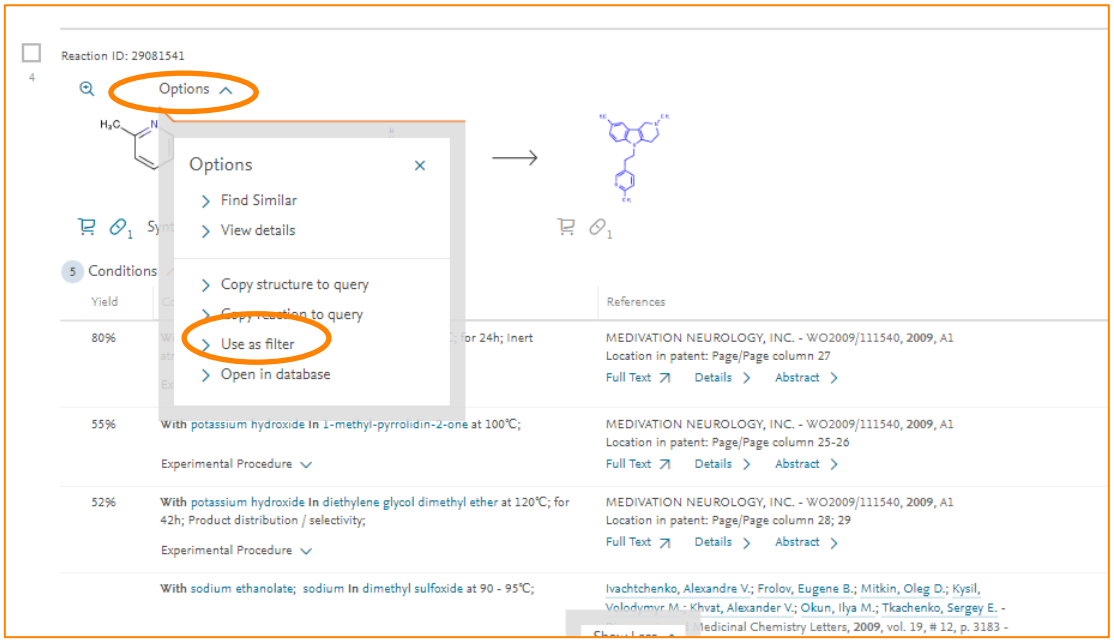


4. Filtering results for specific intermediates or reactants

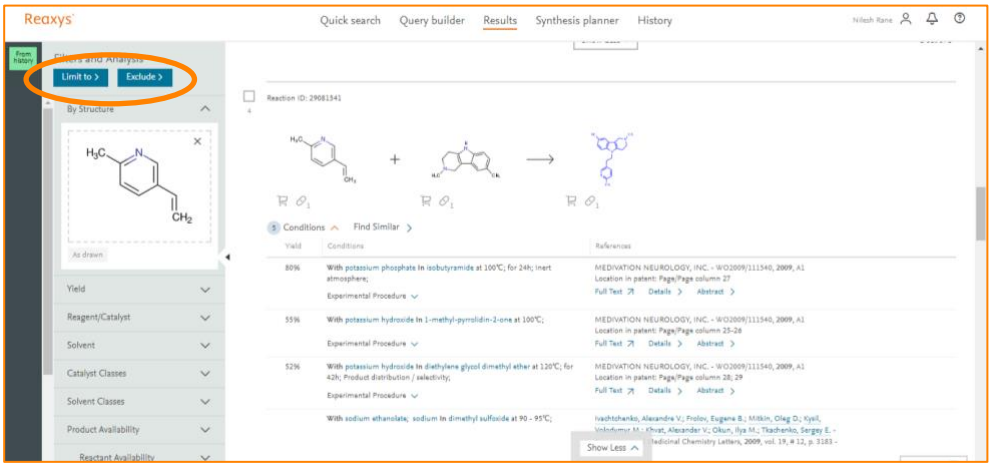
To look through the main results, filtering for intermediates and reactants, click **History** and then click **View** for the first set of results.



Open the **Options** menu for a given reactant and select **Use as filter**. It will automatically add to the filter **By structure**.



Select **Exclude** to view all the reactions that do not involve the selected structure as a reactant. Select **Limit to** to view all the reactions that do involve the selected structure as a reactant.



Further reactions or synthetic strategies can be searches using various options from the **Filters and Analysis** panel.

Further information on using Reaxys can be found in the user guide in the Reaxys Support Center.