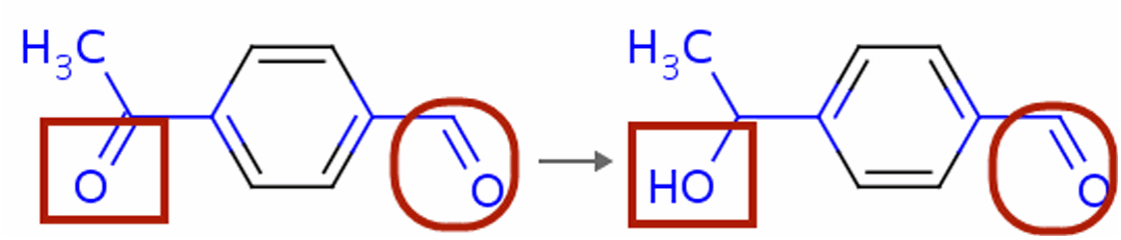
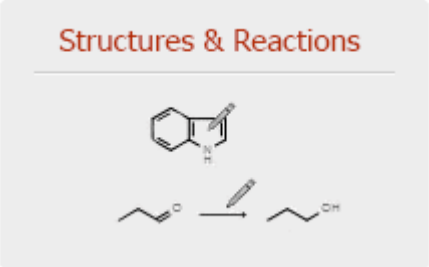
REAXYS®

HOW YOU THINK HOW YOU WORK

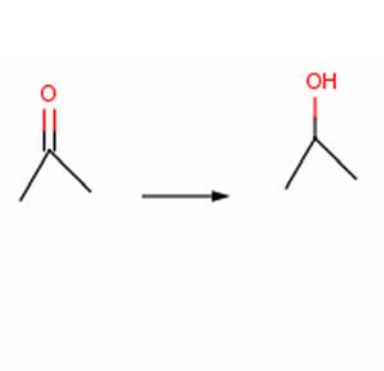


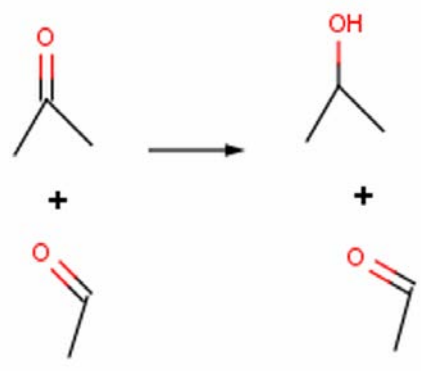
I need to reduce a ketone to a secondary alcohol but I do not want the aldehyde on my reactant to also be reduced to an alcohol. Does Reaxys have any examples of how to do this?

1. Click **Structures and Reactions** from the **Reaxys Start page**. Click the structure box to open the structure editor (MarvinSketch is used here).

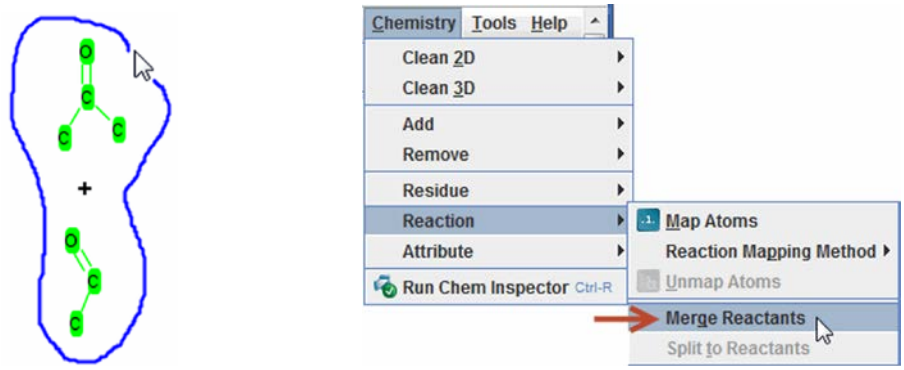


2. Draw the ketone and alcohol fragments. Then add the aldehyde groups. ***Notice that the "+" signs are added.***

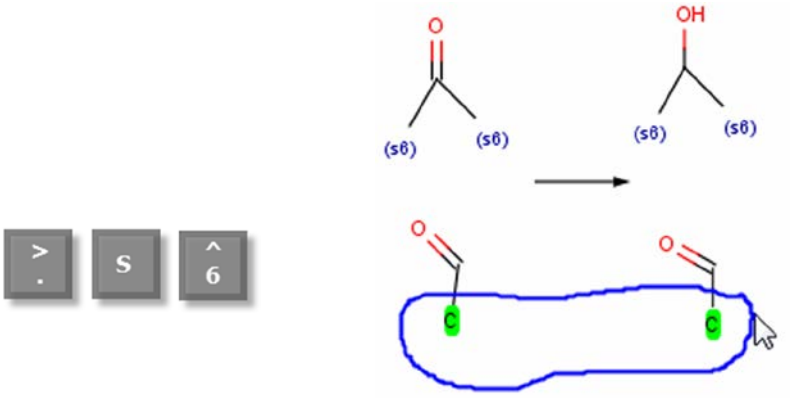




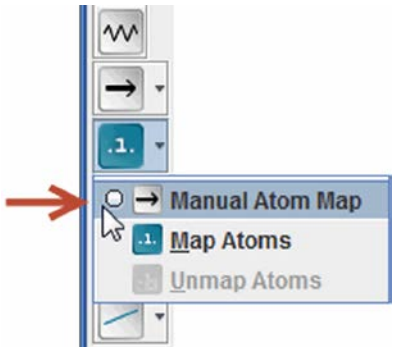
3. Remove the **"+"** signs by first selecting the reactant fragments and then using the **Chemistry menu** to select **Chemistry>Reaction>Merge reactants**. Do the same for the product fragments.

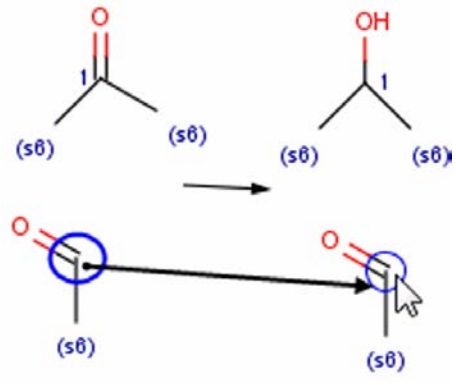


4. The ends of each fragment must be labeled to indicate that those sites are open to substitution. Select the methyls in the top fragments and while they are highlighted in green, type .s6 (one key after the other, not all at once). Do the same for the methyls in the bottom fragments.



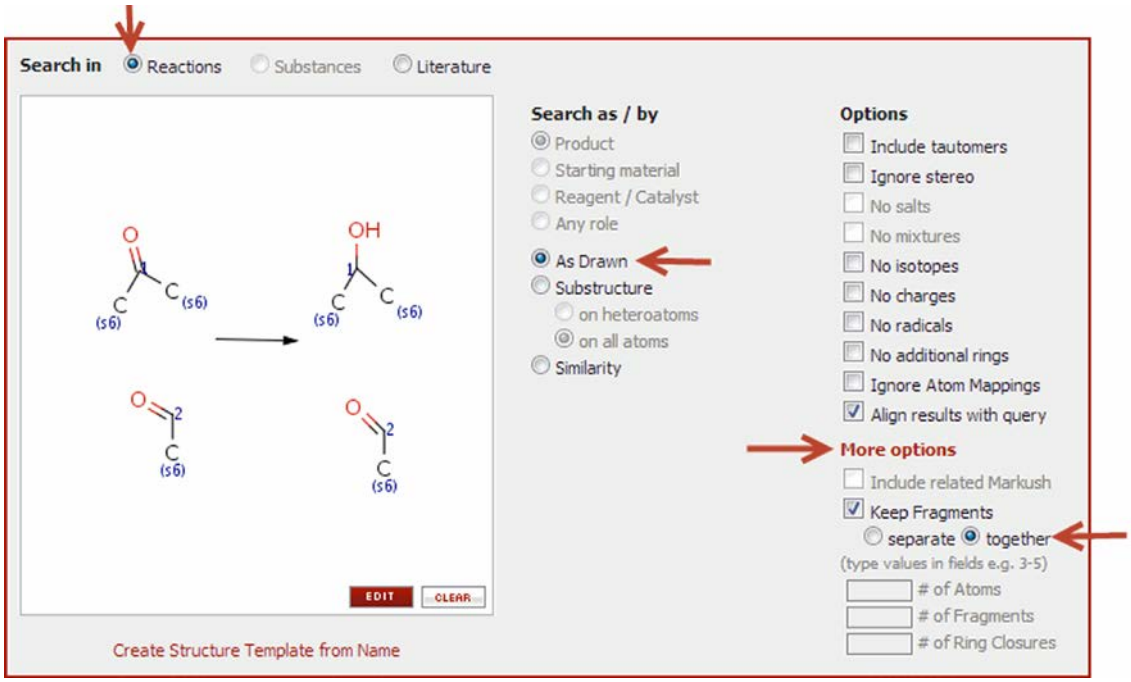
5. Map the fragments to ensure that you retrieve relevant results. Select the Mapping tool, click the relevant carbon on the ketone fragment and drag it to the relevant carbon on the alcohol fragment. Do the same with the aldehyde fragments. The numbers indicate the mapped atom pairs.





6. Transfer the query to Reaxys. Select the **Reactions radio button**, select **As Drawn**, click the **More options** link and select **Keep fragments together**.

The final query looks like this:



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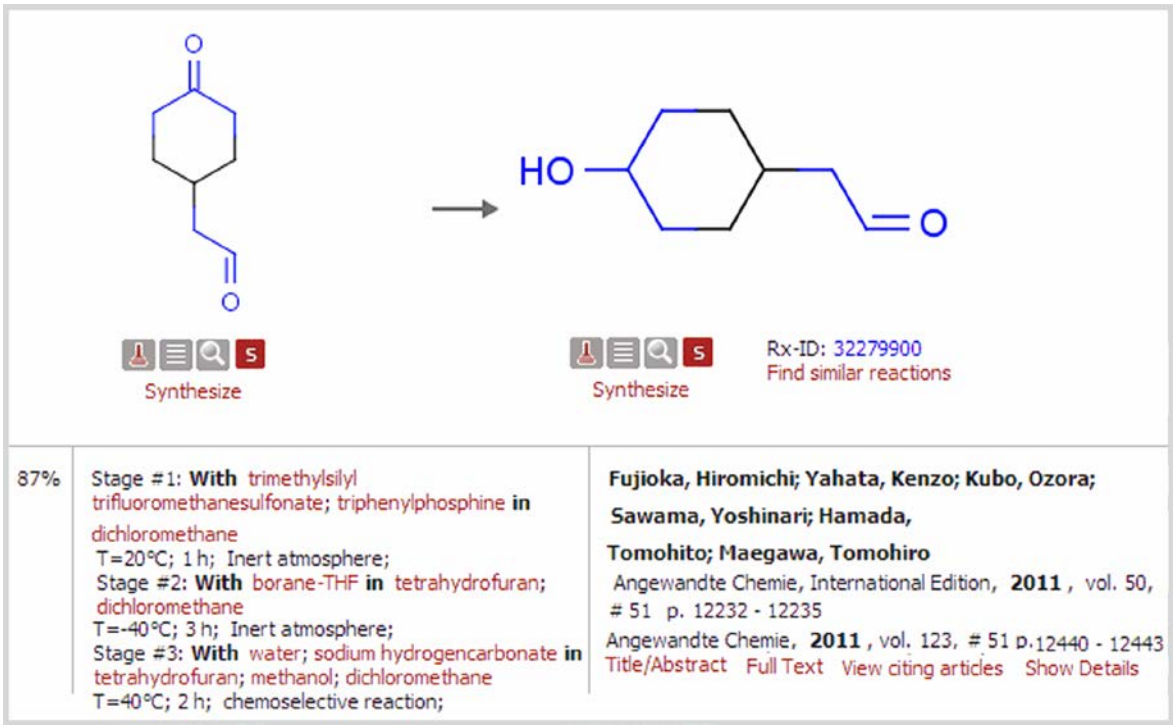
Results:

About 126 reactions are retrieved. For example:



87%	Stage #1: **With** trimethylsilyl trifluoromethanesulfonate; triphenylphosphine **in** dichloromethane T=20°C; 1 h; Inert atmosphere; Stage #2: **With** borane-THF **in** tetrahydrofuran; dichloromethane T=-40°C; 3 h; Inert atmosphere; Stage #3: **With** water; sodium hydrogencarbonate **in** tetrahydrofuran; methanol; dichloromethane T=40°C; 2 h; chemoselective reaction;	**Fujioka, Hiromichi; Yahata, Kenzo; Kubo, Ozora; Sawama, Yoshinari; Hamada, Tomohito; Maegawa, Tomohiro** Angewandte Chemie, International Edition, **2011**, vol. 50, # 51 p. 12232 - 12235 Angewandte Chemie, **2011**, vol. 123, # 51 p.12440 - 12443 Title/Abstract Full Text View citing articles Show Details

Do you have an idea for a workflow example?

Please contact me:

Christine Flemming

c.flemming@elsevier.com

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