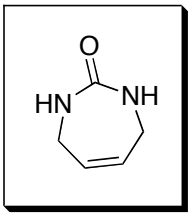
Dr. Peter Wipf

Chemistry 1310/2370 - Synthetic Organic Chemistry

Problem Set 5 (THERESA): Due Date 12/7/09 Name:

Use the THERESA program to answer the following questions.

1.) Perform a search on the structure shown below:

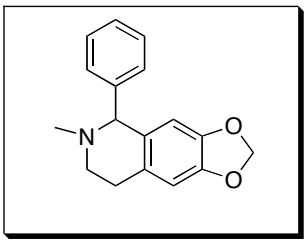


a) Of the first ten suggestions generated by THERESA, which approach do you think is the most viable? Draw the reaction scheme in the space provided (include the starting materials and product as well as a suggested reagent over the reaction arrow).

b) *Briefly* explain what factors made you choose this selection.

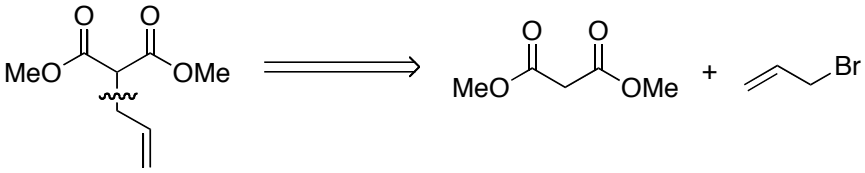
c) Generate a synthesis tree and report for your chosen route. Be sure that the last node in your tree is a commercially available material. Attach the tree and report the problem set.

2. Perform a search on the following structure:

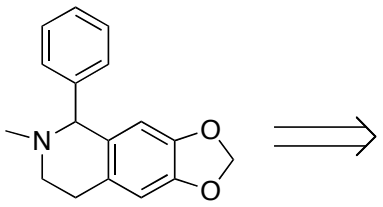


a) Look at the first three suggestions generated by THERESA. Draw the retrosynthetic disconnections represented by the suggestions.

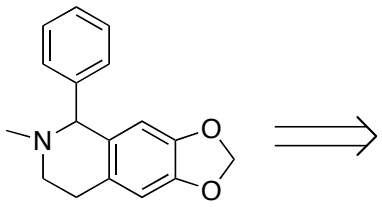
Example for a different system:



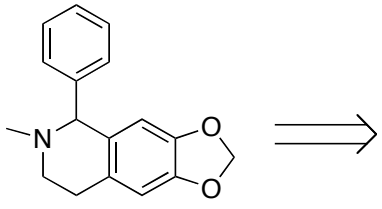
Suggestion 1:



Suggestion 2:



Suggestion 3:



b) Look at the “similar reactions from CCR” for the first three suggestions.

Which disconnection do you favor based on the given precedence? Briefly explain your decision, and draw the reaction scheme from the literature example (as shown in the THERESA window) that best supported your choice.

Look again at the precedence listed for the other two suggestions. Do the examples give good support for those suggestions? Briefly explain why or why not.

c) All three suggestions look like they start with commercially available material. Yet, suppliers have just announced a shortage of the starting material depicted in Suggestion 3! Your friend (a graduate student) is determined to make multi-gram quantities of the target compound following this route. You are called to help by performing the following tasks:

i.)Resubmit the starting material as a new query.

ii.)Choose a viable route for synthesis of the starting material based on the first ten suggestions generated by THERESA.

iii.) Generate a complete synthesis tree starting with the target compound and ending with the new starting materials you would need for this route. Make sure the last nodes of the tree are commercially available materials. Staple a copy of the tree to the problem set.