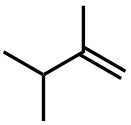
Retrosynthesis

Please ensure that you have completed the "Review of Fundamental Functional Group Interconversions" Worksheet prior to completing this "Retrosynthesis" Worksheet.

1. Reference your completed "Review of Fundamental Functional Group Interconversions" Worksheet to conduct a retrosynthetic analysis on the shown target molecules using the template provided. Draw your starting material in the box and define its key functional group. Above each retrosynthesis arrow, define the reagents/reaction conditions needed. Below each retrosynthesis arrow, classify each reaction type as acid-base, substitution, elimination, or addition to a π bond.

Note: this page is exclusively asking you about one step/reaction processes.

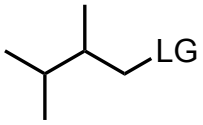


target alkene

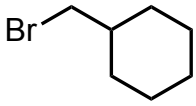
any appropriate E2 base (ex: $NaNH_2$)

elimination (E2)

alkyl halide or other leaving group (LG)

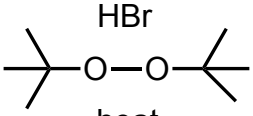


starting material



target alkyl halide

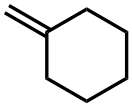
HBr



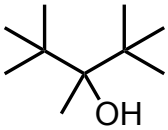
heat

addition (Anti-Markovnikov)

alkene



starting material



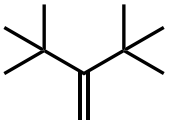
target alcohol

catalytic H_2SO_4

H_2O

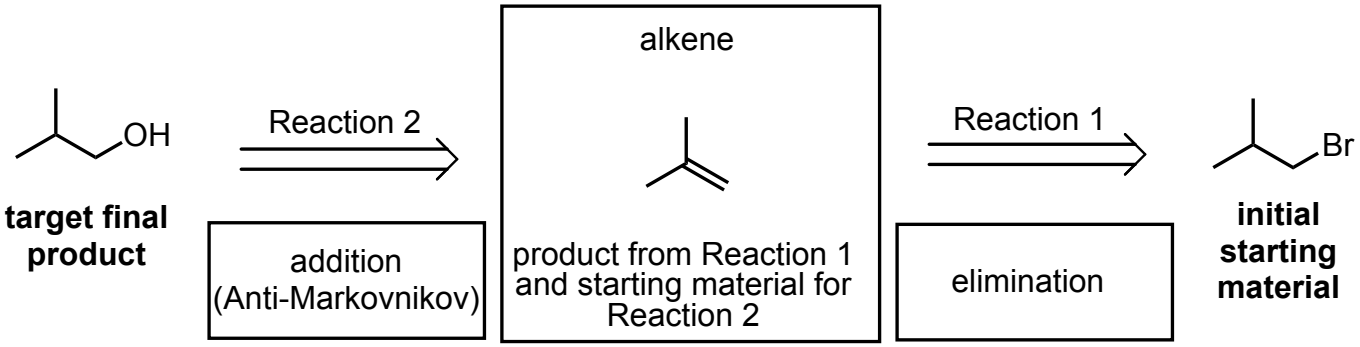
addition (Markovnikov)

alkene



starting material

2. Perform a retrosynthetic analysis on the target final product using the template and guiding questions, labeled as parts a-f.



a) Were any new carbons based groups added to the target final product? No

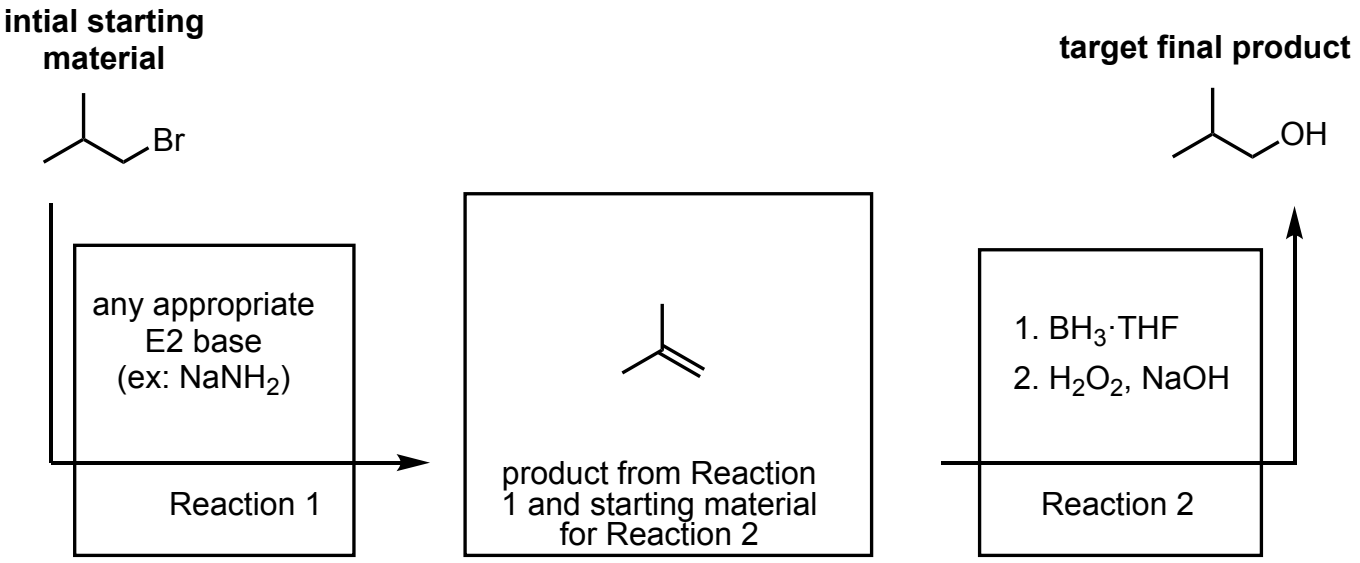
b) What new functional group(s) are present in the target final product? Are they at a more or less substituted position? Alcohol at the less substituted position

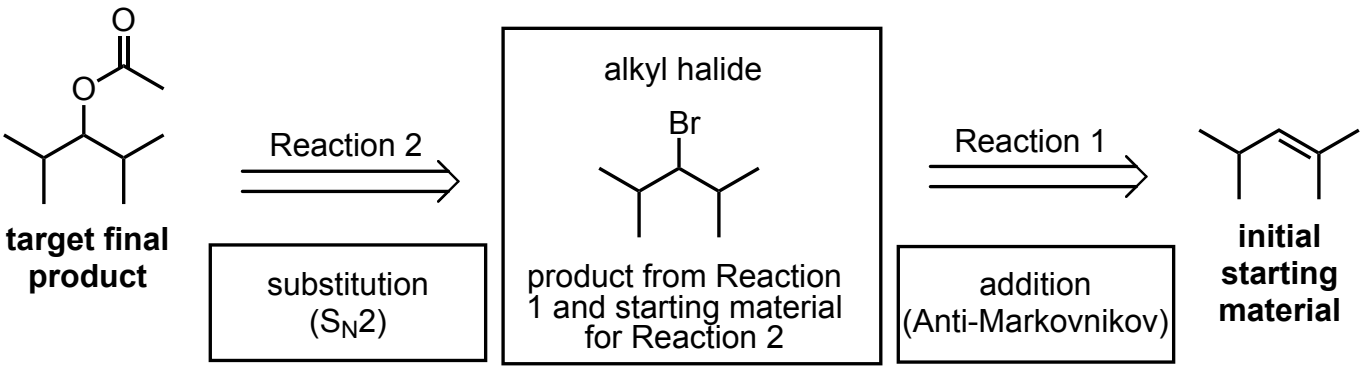
c) What type of reaction (ex: substitution, elimination, etc.) could form this new functional group? Place your answer in the box below the retrosynthetic arrow labeled as "Reaction 2".

d) What type of starting material is needed to enable Reaction 2? Draw it in the middle box.

e) What type of reaction could enable the initial starting material to tranform into the boxed molecule? Place your answer below the retrosynthetic arrow labeled as "Reaction 1".

f) Use the work above to help you provide a forward synthesis, shown below. Fill in the boxes with the missing reagents and products needed to complete each series of reactions.





a) Were any new carbons based groups added to the target final product? Yes

b) What new functional group(s) are present in the target final product? Are they at a more or less substituted position? Ester at a less substituted position

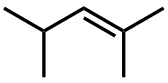
c) What type of reaction (ex: substitution, elimination, etc.) could form this new functional group? Place your answer in the box below the retrosynthetic arrow labeled as "Reaction 2".

d) What type of starting material is needed to enable Reaction 2? Draw it in the middle box.

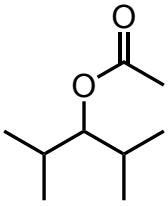
e) What type of reaction could enable the initial starting material to tranform into the boxed molecule? Place your answer below the retrosynthetic arrow labeled as "Reaction 1".

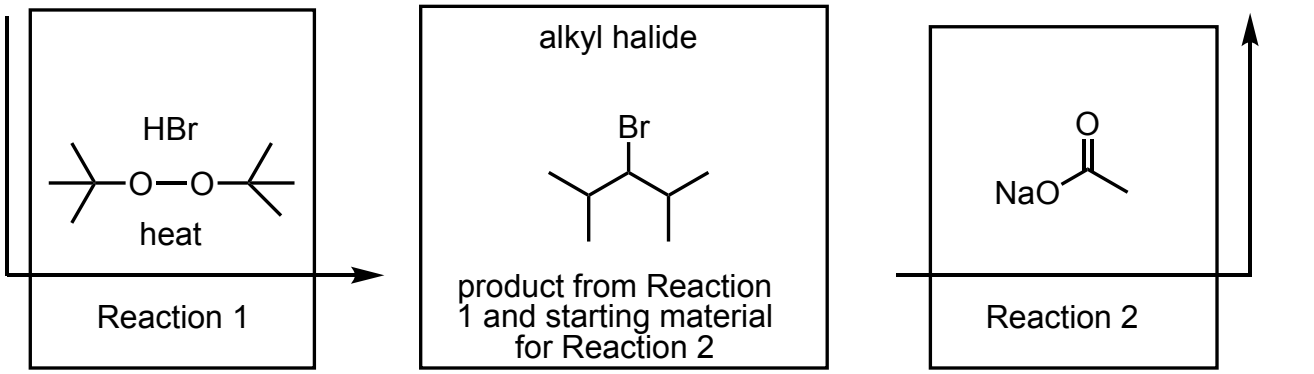
f) Use the work above to help you provide a forward synthesis, shown below. Fill in the boxes with the missing reagents and products needed to complete each series of reactions.

intial starting material



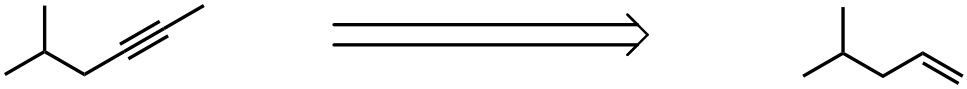
target final product

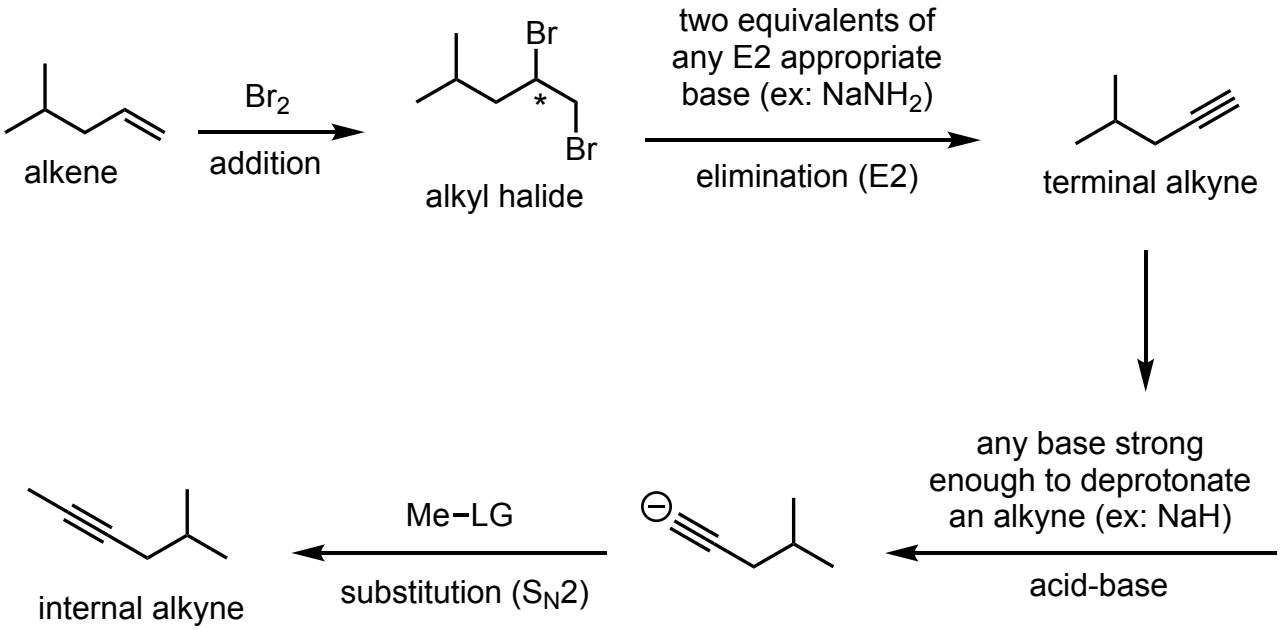




3. Propose a successful forward synthetic route for the formation of the shown target final product from the shown initial starting material.

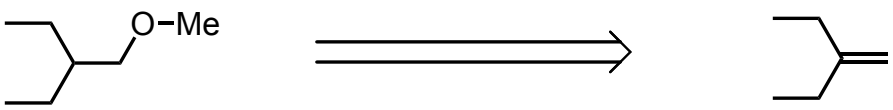
target final product **initial starting material**

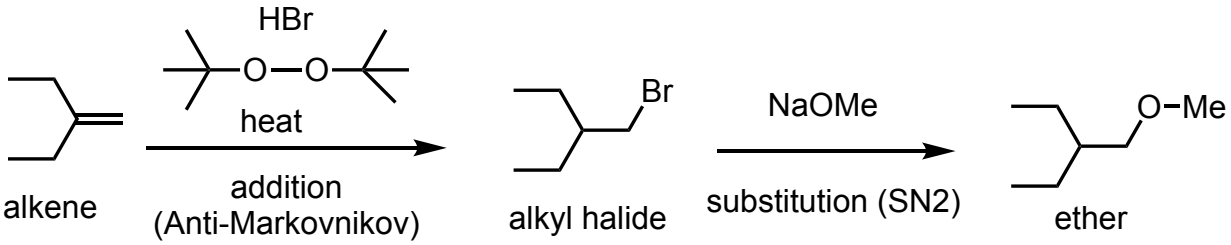


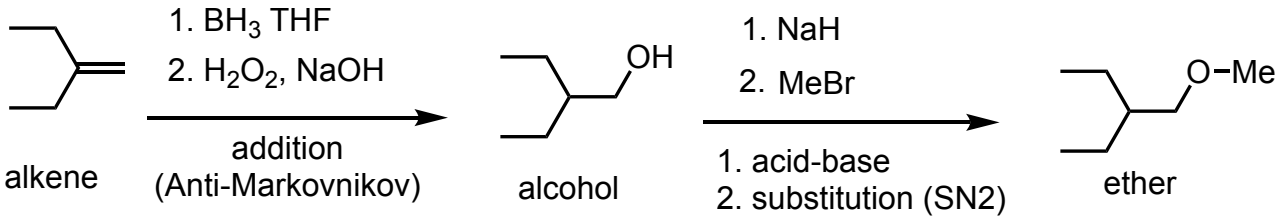


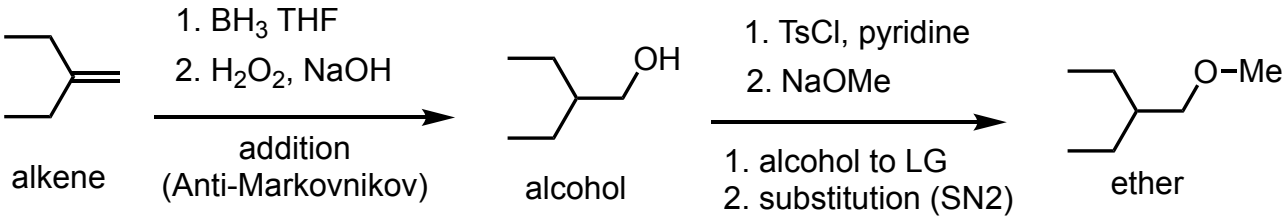
4. Sometimes, there is more than one feasible synthetic pathway. Propose two successful forward synthetic routes for the formation of the shown target final product from the shown starting material.

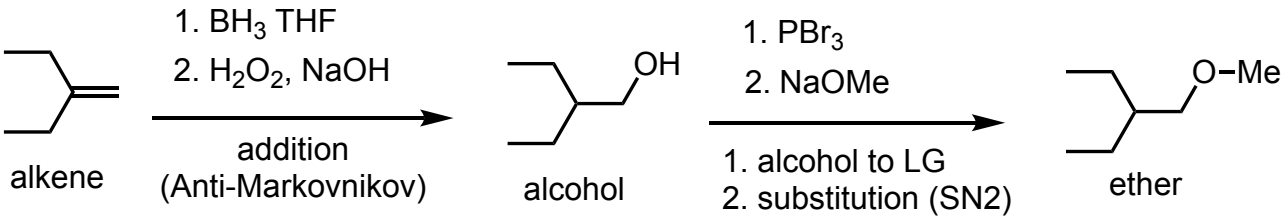
target final product **initial starting material**



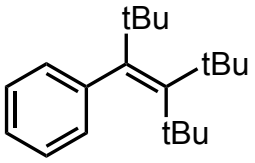






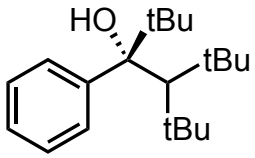


5. CHALLENGE QUESTION! You are a chemist tasked with needing to synthesize the target final product as part of a new pharmeceutical drug discovery project. More specifically, you need to devise the most inexpensive, efficient, and environmentally friendly synthetic pathway. (*Note: these last two goals can generally be achieved by ensuring that your plan employs the smallest number of reactions needed.*) You are given access to the chemicals below at the shown prices. What is your proposed plan?

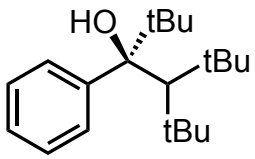


target final product

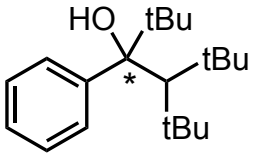
chemicals available to you in your stockroom



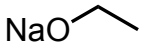
$200 / gram

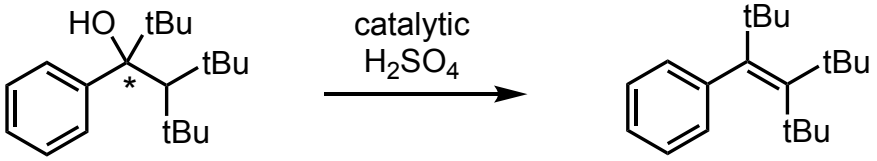


$200 / gram



$30 / gram

H_2SO_4	PBr_3	TsCl	pyridine	
$0.03 / gram	$0.15 / gram	$1 / gram	$0.40 / gram	$0.60 / gram



The acid catalyzed dehydration of either enantiomer alcohol starting material successfully forms the target final product. Thus, the reaction will also be successful when using the cheaper racemic alcohol starting material. This is the most inexpensive, efficient, and environmentally friendly synthetic pathway to create the target final product.

The pathway of tranforming the alcohol to an alkyl bromide, followed by E2 elimination is succcessful at making the product. However, it is more expensive and requires two overall reactions.

The pathway of tranforming the alcohol to a tosylate leaving group, followed by E2 elimination is succcessful at making the product. However, it is more expensive and requires two overall reactions.