Pandemic-Modified Lab Report for Research-Module Week 1: Scheme 1/Week 1 Lab Report:

1. Download the docx written procedure for Scheme 1 reaction (**1** → **3a**).
2. Insert listing of chemicals used; show your mole calculations; identify limiting reactant; and show your theoretical yield calculation. (As per normal report.)
3. Note: assume you used crotonic acid **1a** and made product **3a** (and minor isomer **4a**).
   - Even though in the actual video, I actually did it using 2-pentenoic acid **1b**! ☺
   - But the data analysis, NMR analysis, and derivative products from Week 2 will involve **3a**, not **3b**. And the GC-MS had a problem so that I couldn't analyse **3b**.
     - The NMR analyses involving **3a** are also much easier than for **3b**.
   - So it will work much better for you (and for me) to just work with and analyze known data, NMR's, and GC's for **3a** rather than **3b**.
4. Insert observations as they occur; or any changes in procedure.
   - (A different font or a different color would be nice, so your inserts stand out from copied text! ☺)
5. Include final mass, % yield calculation.
6. Make sure that all structures are drawn explicitly.
   - As always for a synthesis style report, you'll want to draw out the reactants and the products. In this case, be sure you draw the **actual** crotonic acid reactant and product **3a** in your reaction.
   - None of your pictures should have an "R1": you should illustrate each structure with your actual R1 group drawn, whether that's methyl or phenyl or 4-methoxyphenyl or whatever.
7. Show all calculations. (Including any mole => mass for reactants, or mass => mole for products)
8. Calculate mass yields, and percent yields, etc., for product **3**.
9. Include presentation and data summary of your NMR-**3**
   - The NMR is attached as the last page of this document.
   - Be sure to draw your structure, and then provide an abbreviated summary report. This should include a listing of chemical shifts, integrations, and splittings, and a matchup-assignment between signals and hydrogens in the molecule.
   - **Note: you do not need to include impurities/solvents/contaminants in the abbreviated NMR summary report**.
   - Some of the splitting will be more complex than you've previously experienced, due to the impact of chirality. See NMR-processing discussion. I won't be very concerned about how you report some of these. ("m" for multiplet, or "dd" for doublet-of-doublet might be OK…)
10. Include your data summary for GC-MS data for **3a** and **3b**. The GC-MS data summary is included at the back of this document.
11. Include a results/data/discussion/analysis section. The analysis/discussion section needs to address what the yield information told you, and what the NMR and GC-MS data tells you about both the success and the efficiency of your reaction, and the purity of your product **3**.
12. The results/data/discussion/analysis section should summarize what the mass/yield/NMR/GC-MS data is, and what conclusions can be drawn from them. Just attaching the NMR's and GC-MS's without discussing or showing that you understand them will not be good. What is the summary for the key non-aromatic C-H hydrogens in your NMR? What is your GC-retention time? Between the NMR and the GC, did it look like the product **3** was formed successfully, and does it look reasonably clean? Or is it obviously significantly contaminated?
13. Answer the post-lab questions on the following two pages, and include in your report.