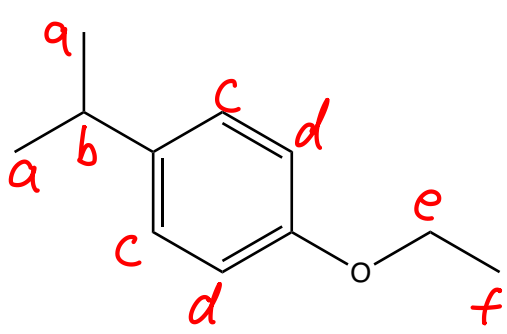
V3 Answers

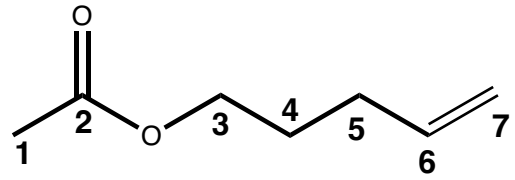
Chem 360-Jasperse Test #2 NMR, IR Version 3.

1. Predict the ^{1}H NMR spectrum. Include the source (CH_3-1, etc); approximate chemical shifts (1's, 2's, etc.); integration (1H, 2H, etc.); and splitting (either list the number of lines, or else use letters: "s" for singlet; "d" for doublet etc.). If signals are symmetry equivalent, do not list them twice.



Source	Chem Shift	Integration	Splitting
CH_3-a	1's	6H	2 = d
CH-b	2's	1H	7 = m
CH-c	7's	2H	2 d
CH-d	7's	2H	2 d
CH_2-e	3's	2H	4 q
CH_3-f	1's	3H	3 t

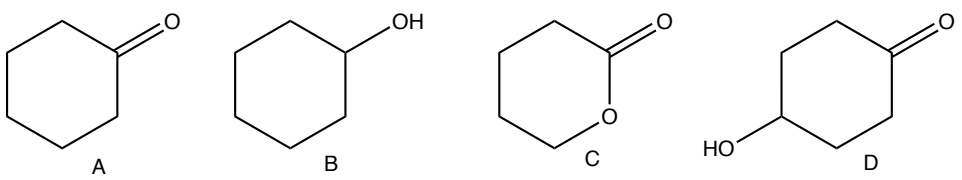
2. Predict the ^{13}C NMR spectrum. Include the approximate chemical shifts (220-160, 160-100, 100-50, or 50-0) and the splitting if a coupled carbon NMR was taken (can either use letters, q, t, d, s, or else number of lines).



Source	Approximate Chem Shift	Splitting
C1	0-50	q
C2	220-160	s
C3	100-50	t
C4	50-0	t
C5	50-0	t
C6	160-100	d
C7	160-100	t

3. Match the following structures with the listed feature IR signals. (Write the letter of the structure by the IR signal):

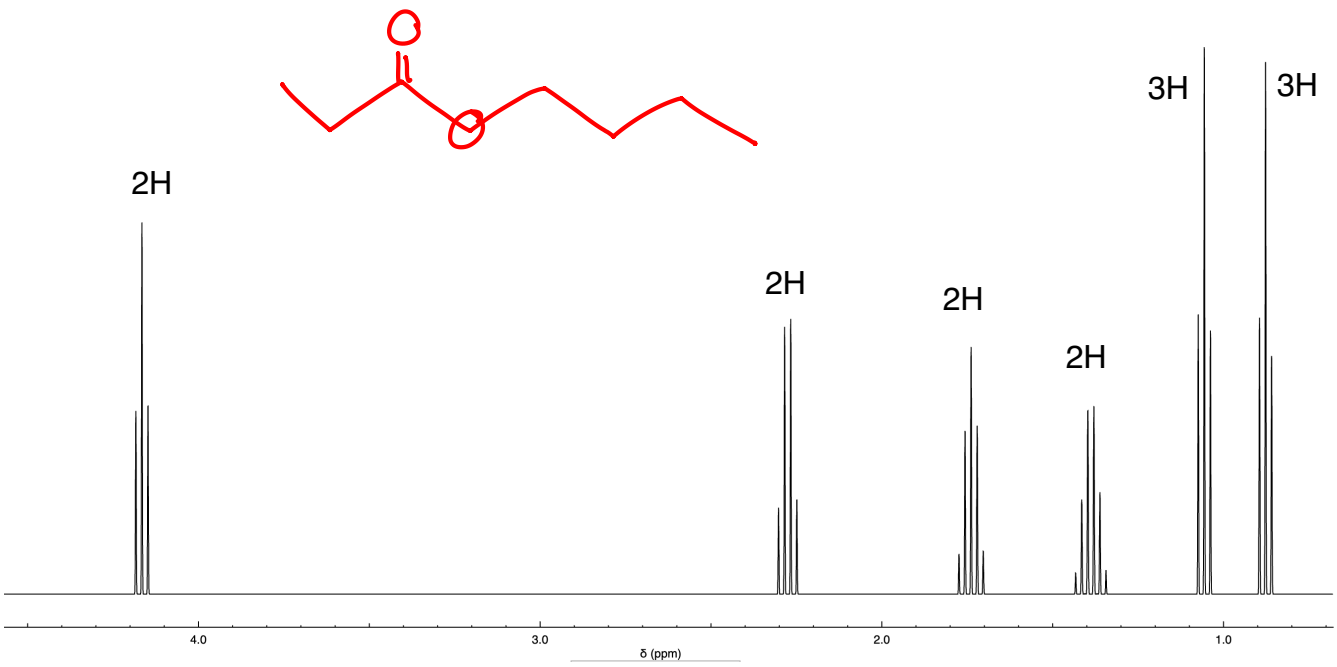
1) 1710 A 2) 3300-3400 B 3) 3300-3200, 1710 D 4) 1745 C



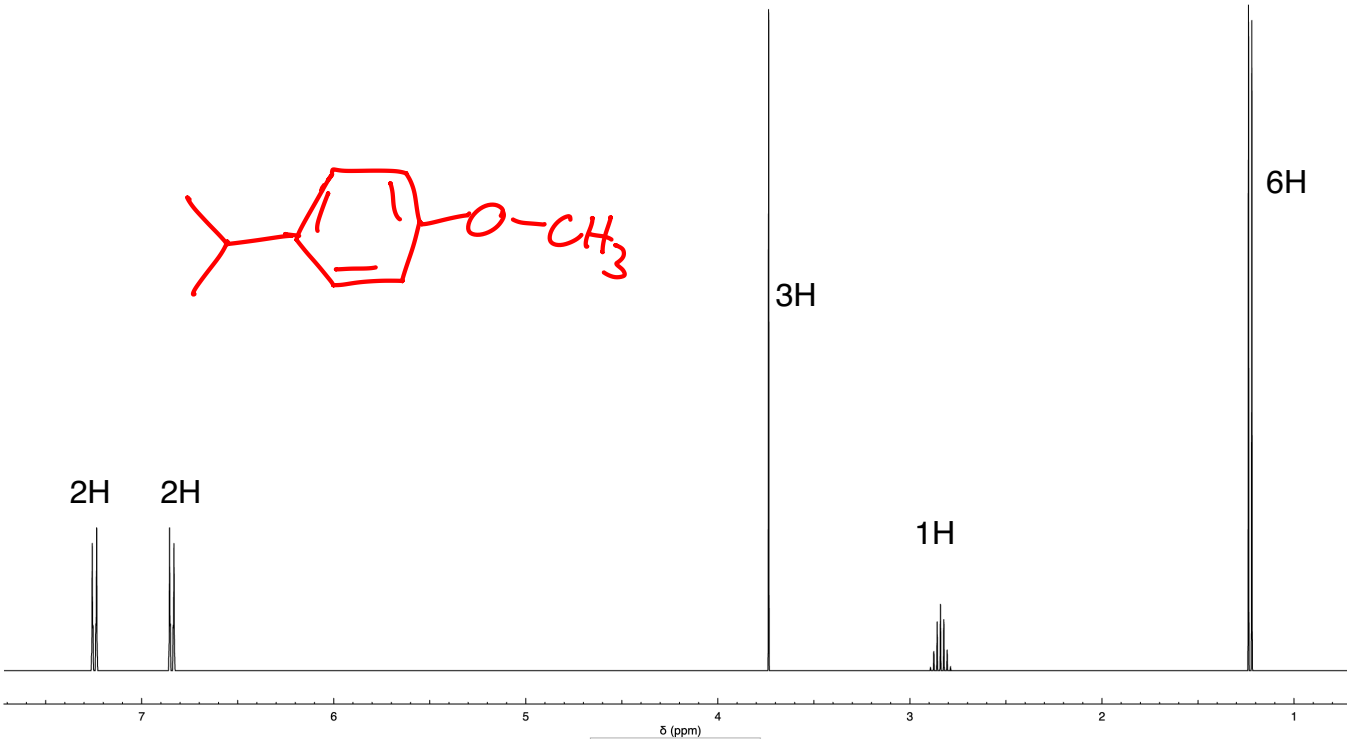
For the remainder of the test, solve the structures for the following. If you get a structure perfect, you will get full credit. If you do not get a structure perfect, you may still get some partial credit. Thus, it is in your interest to show some of you work, make a structure, or tell me what you know for sure.

4. $C_7H_{14}O_2$ IR: 1745

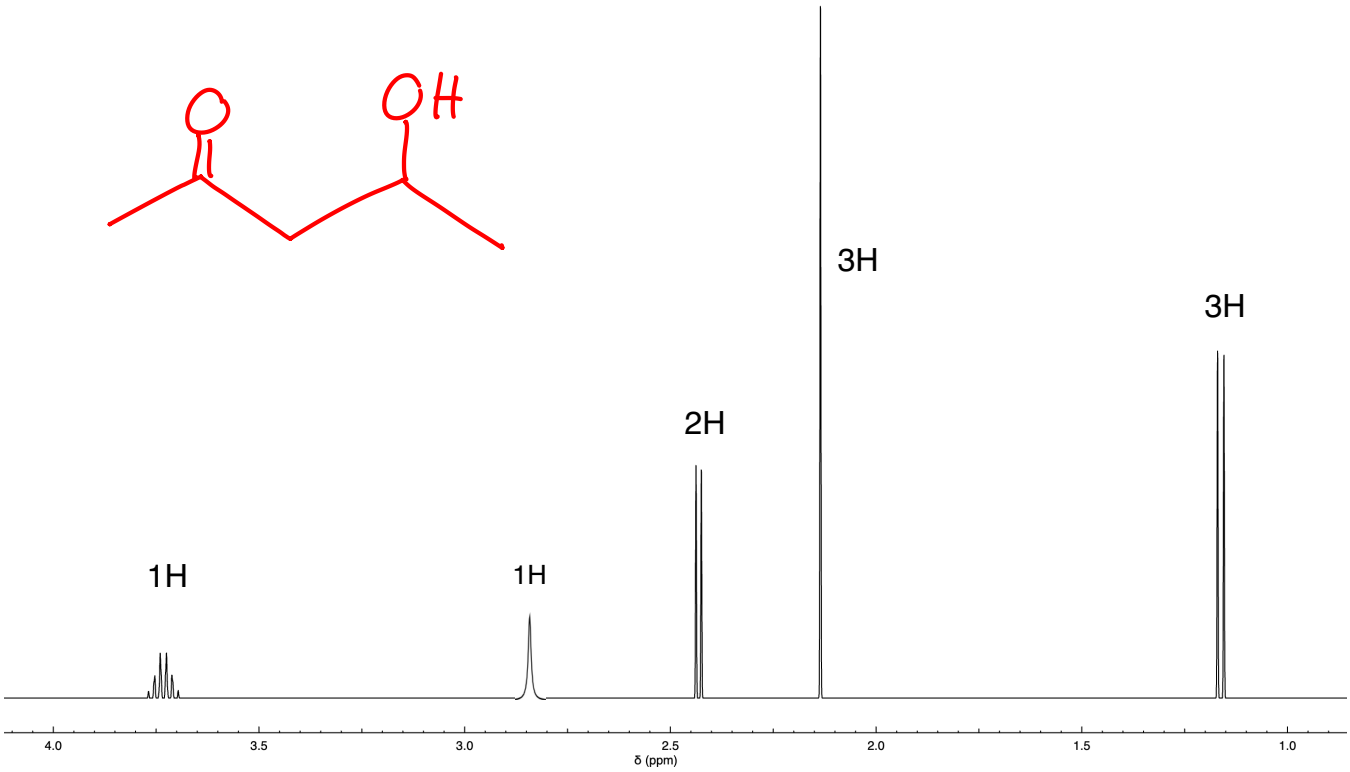
^{13}C NMR: 175 (s, short), 65 (t), 32 (t), 28 (t), 19 (t) 14 (q), 9 (q)



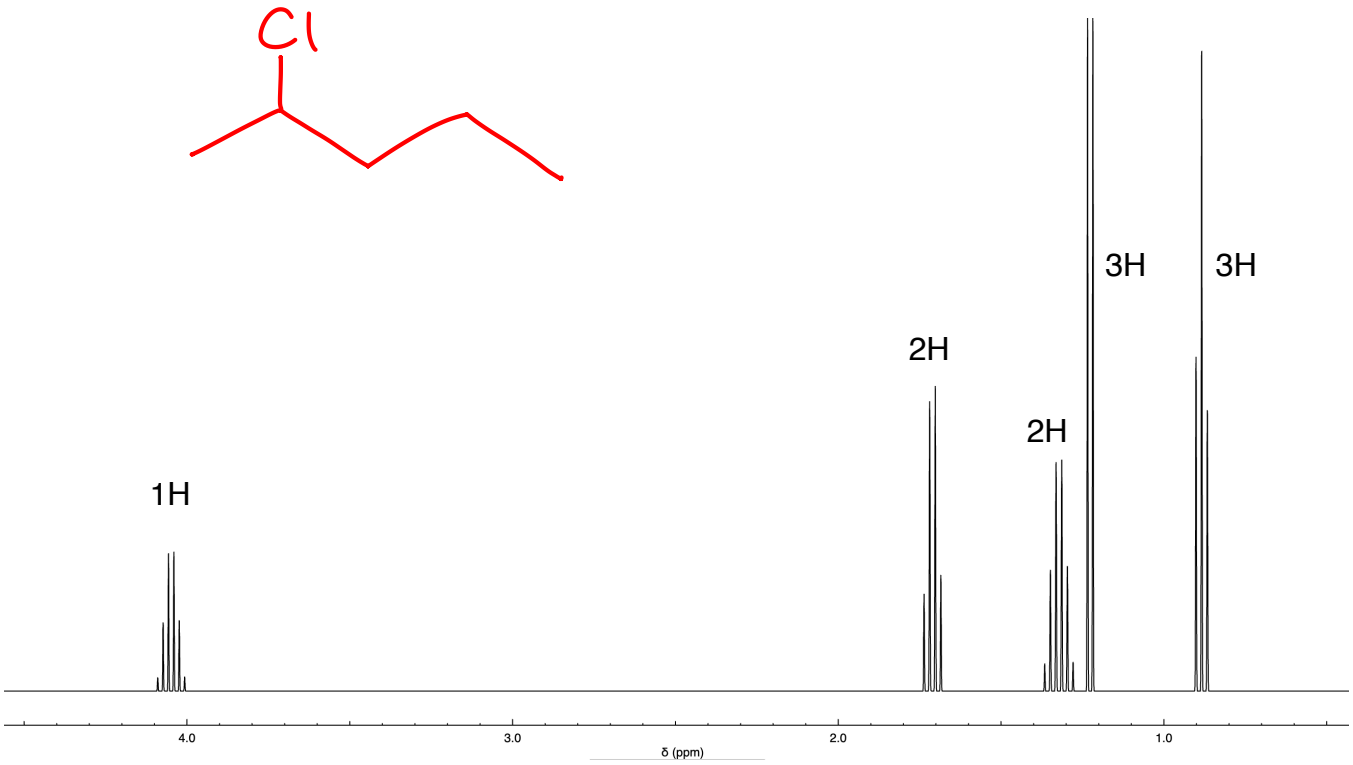
5. $C_{10}H_{14}O$ IR: nothing interesting ^{13}C: 158 (s), 141 (s), 128 (d), 114 (d), 65 (q), 33 (d), 24 (q, tall)



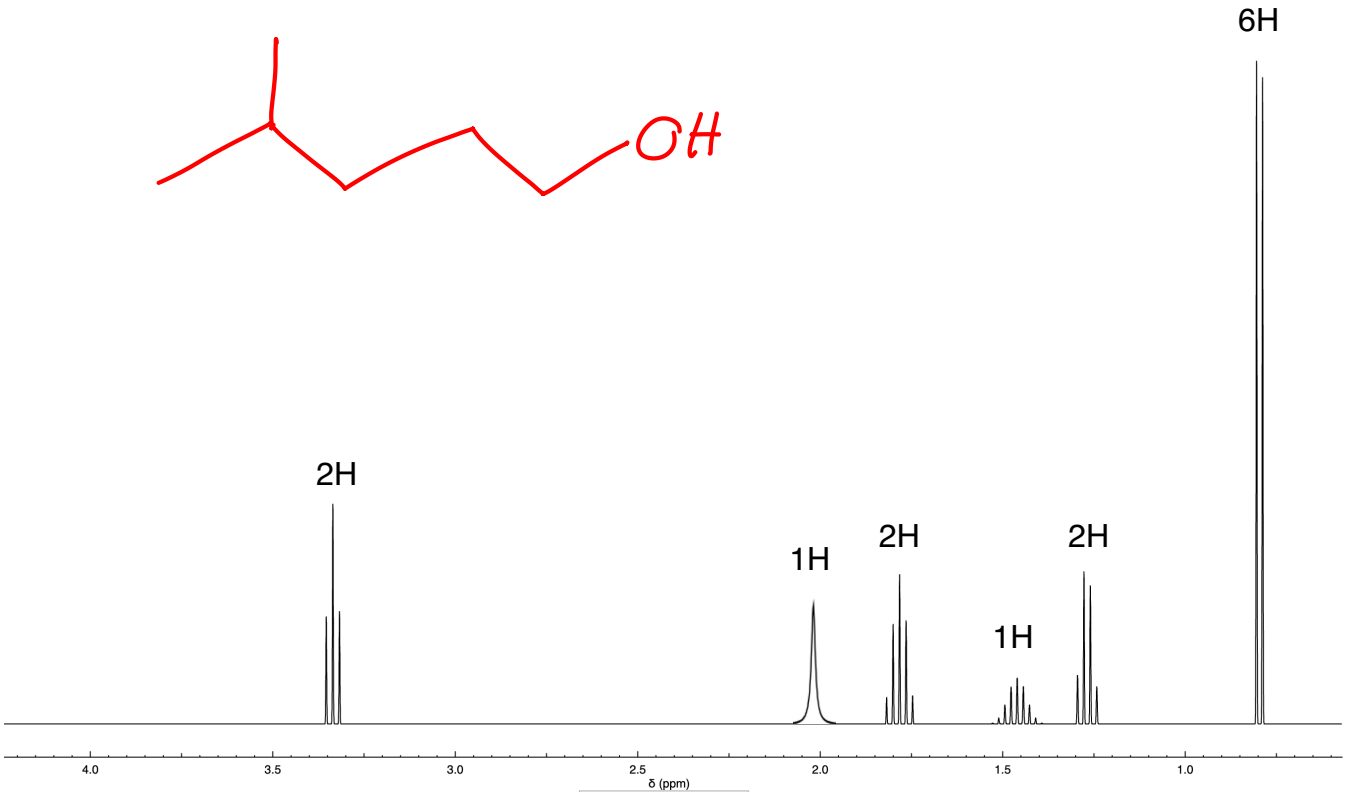
6. $C_5H_{10}O_2$ IR: 3300-3200, 1710
^{13}C: 210 (s), 65 (d), 40 (t), 30 (q), 23 (q)



7. $C_5H_{11}Cl$

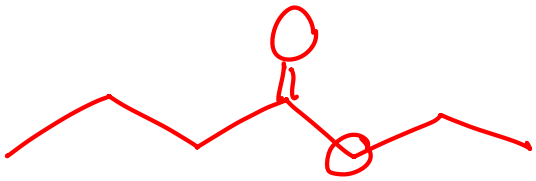


8. $C_6H_{14}O$ IR: 3300-3200
^{13}C: 63 (t), 34 (t), 30 (t), 27 (d), 22 (q, tall)

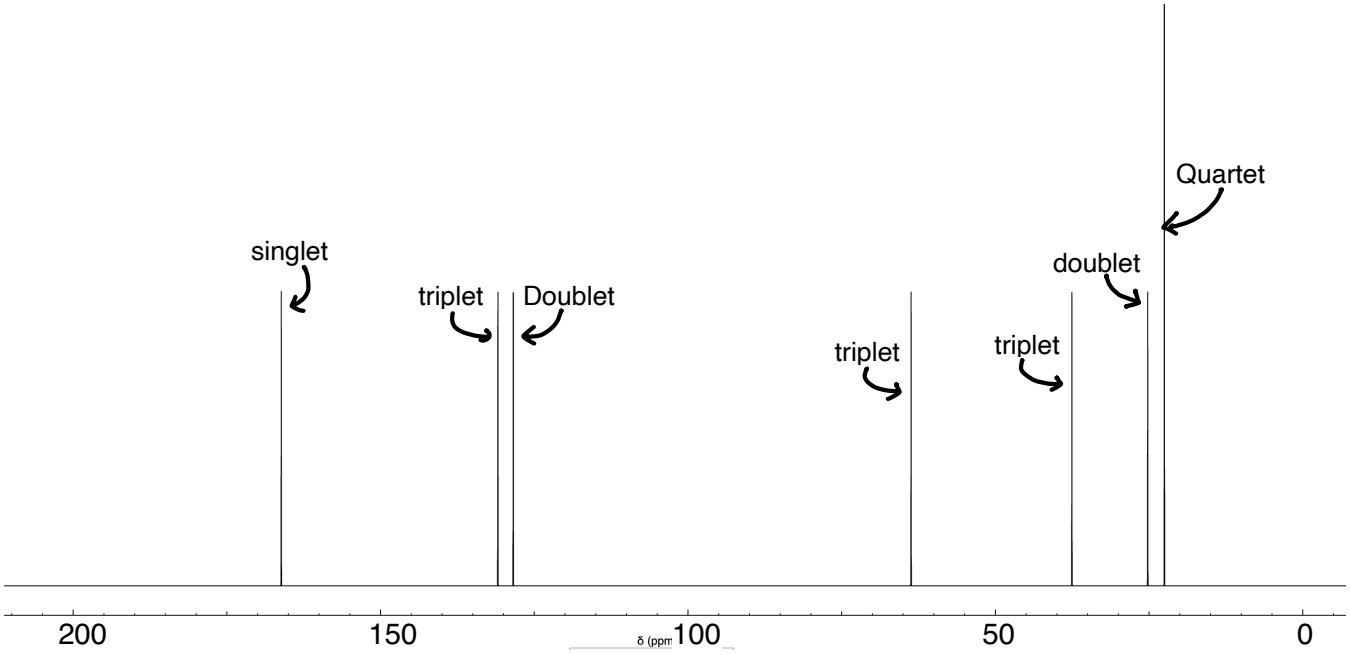


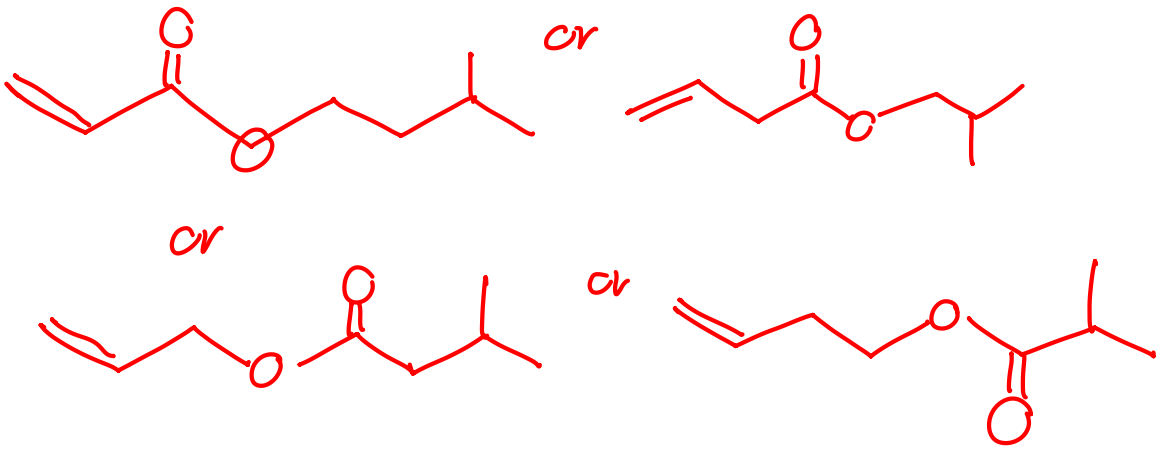
9. $C_6H_{14}O_2$ IR: 1745
13C NMR: 172 (s), 61 (t), 36 (t), 19 (t), 14 (q), 13 (q)

0.92, 3H, triplet
1.15, 3H, triplet
1.62, 2H, sextet
2.22, 2H, triplet
4.10, 2H, quartet



10. $C_8H_{14}O_2$
    - The spectrum displayed is a "decoupled" 13-C NMR spectrum. (No splitting)
    - But beside each coupled peak is a label that tells whether the carbon would be a singlet, doublet, triplet, or quartet **if** a "coupled" 13-C NMR had been obtained.
    - Four different answers are all plausible for this.





- I have not, accidentally or intentionally, seen copies or parts of the test in advance, including online. In the event that I did, I will report this to the instructor as soon as possible.