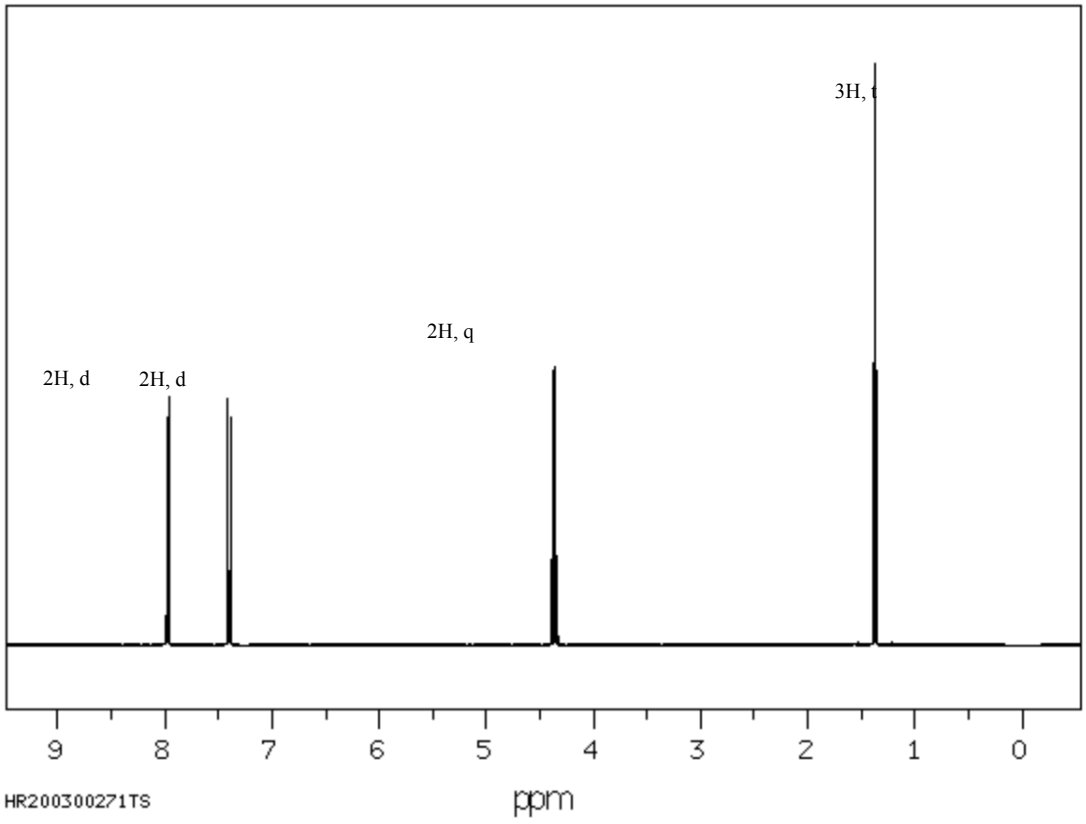
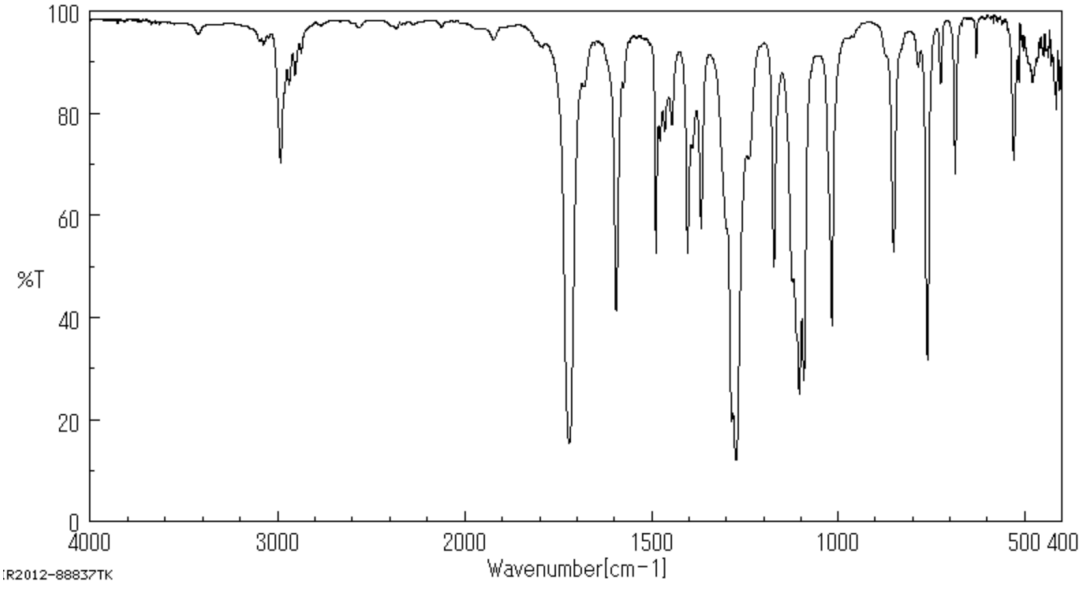
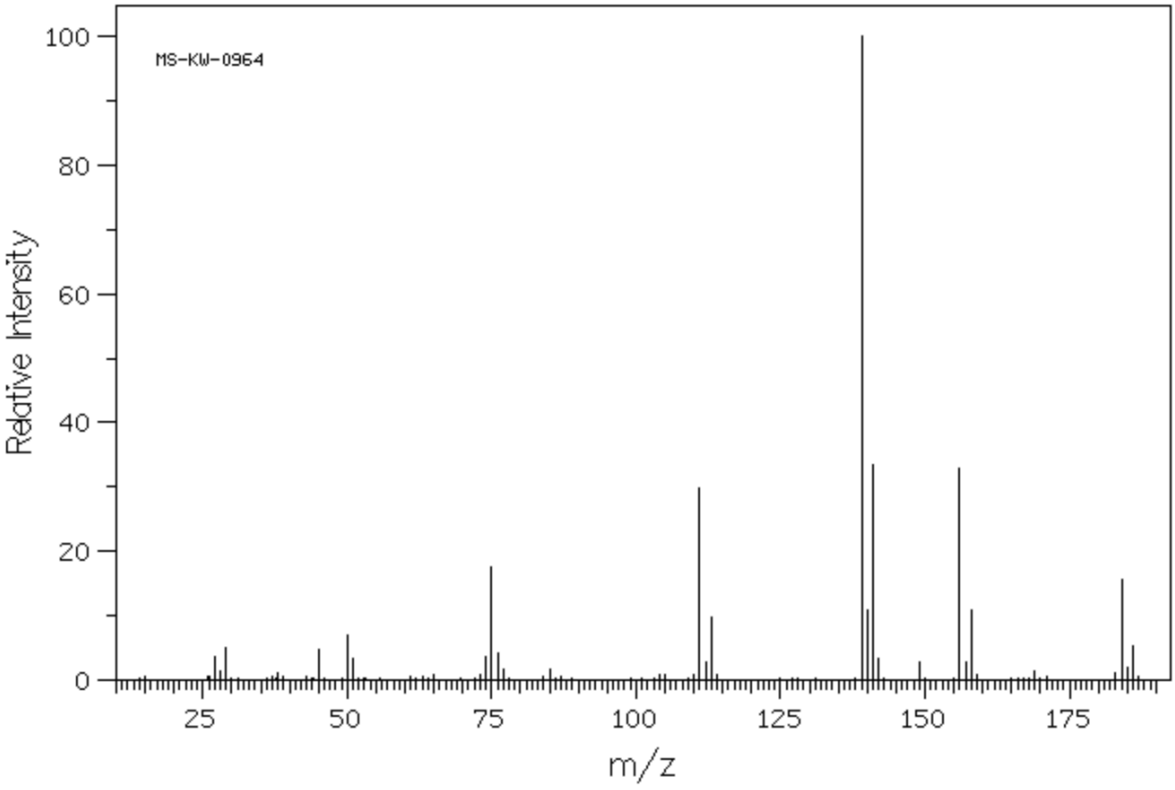
Ch41b 2018 - NMR Problem Solving Session

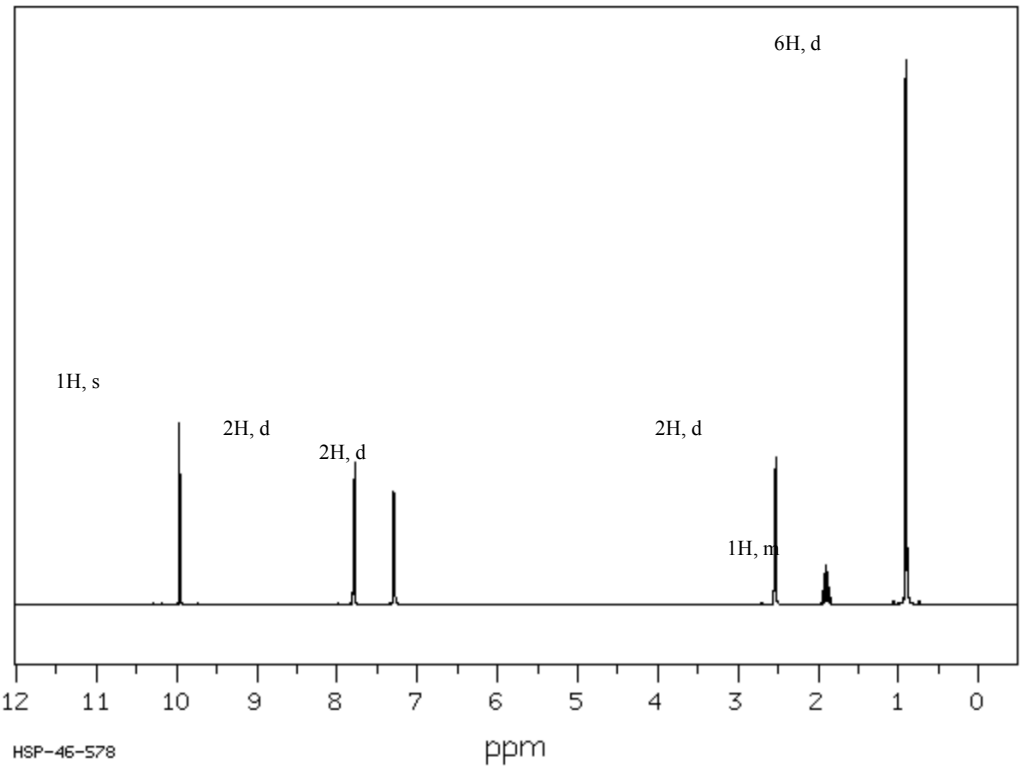
1. An unknown compound has 9 carbons and 9 protons. The molecular ion has an *m/z* of 184. Using the data below:
   - Identify the molecular formula of the unknown compound.
   - Determine the structure of the unknown compound.
   - Identify the fragment that gives rise to the base peak and the fragment that gives rise to the peak at *m/z* = 141. Hint: consider the ratio of the heights of these peaks.

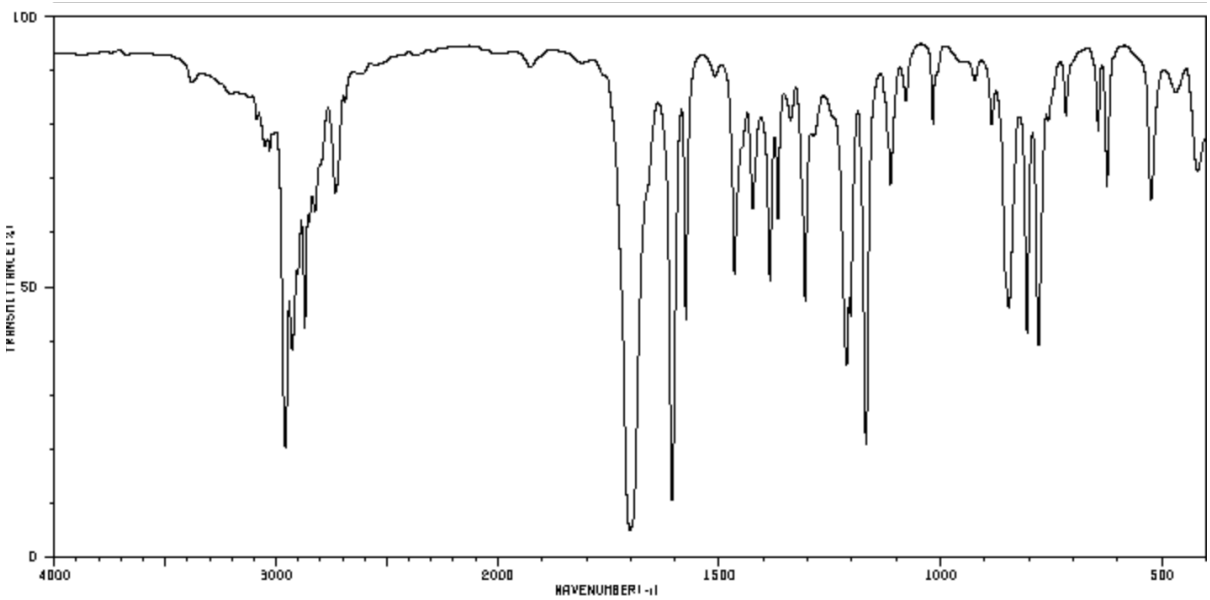


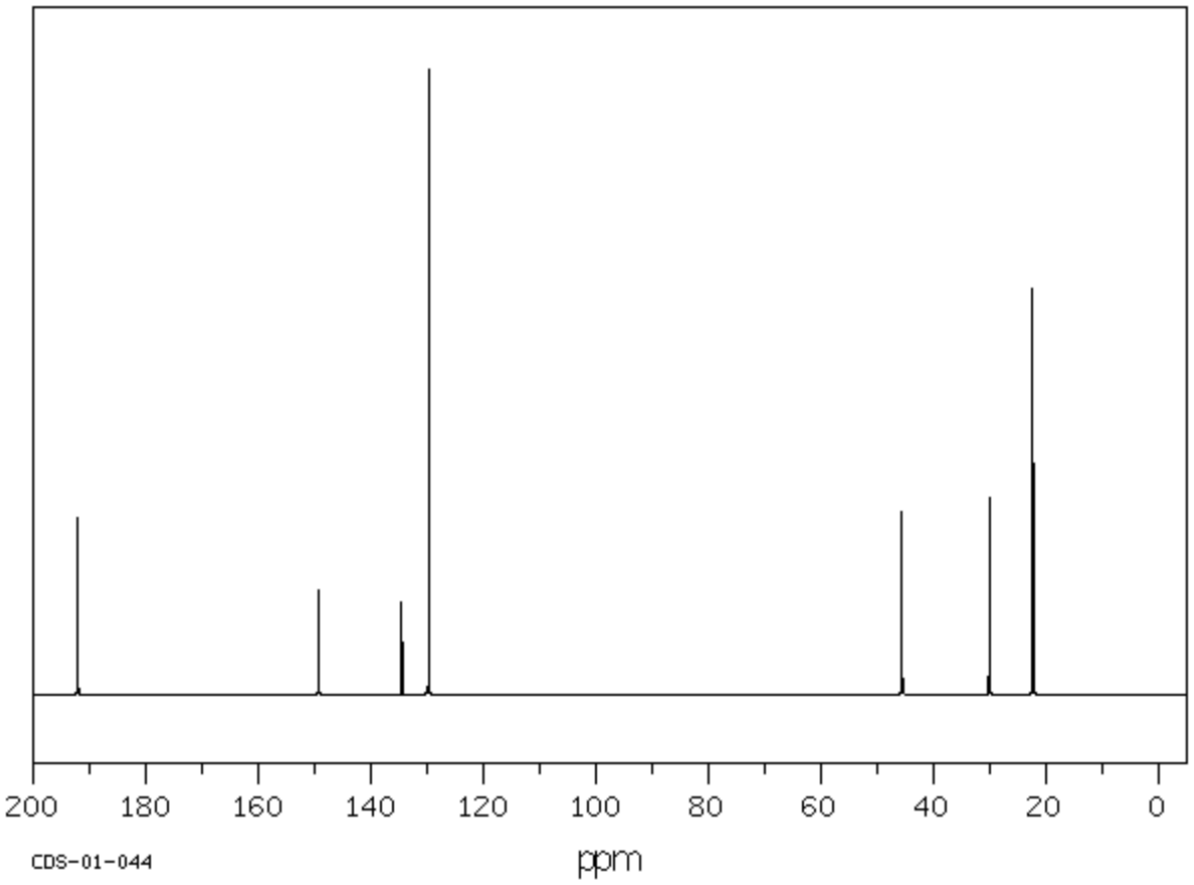



MS-KW-0964
Relative Intensity
100
80
60
40
20
0
25
50
75
100
125
150
175
m/z

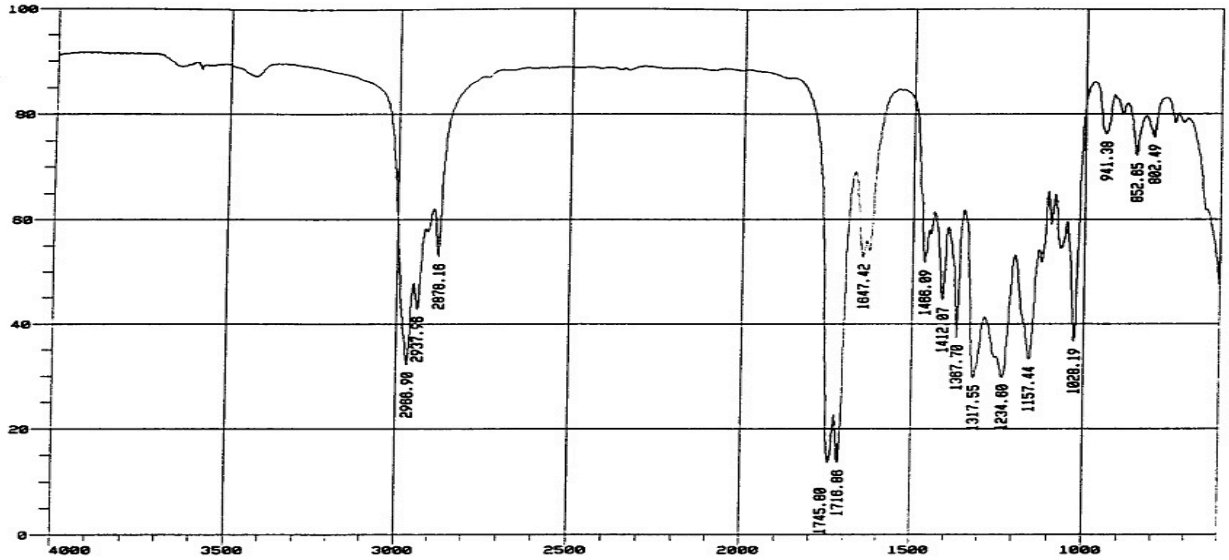
2. An unknown compound has the molecular formula $C_{11}H_{14}O$. Use the following data to:
    - Identify the molecular structure of the unknown compound.
    - Assign the following peaks in the ^{13}C NMR spectrum:
        - δ 192 ppm
        - δ 45 ppm
        - δ 30 ppm
        - δ 21 ppm

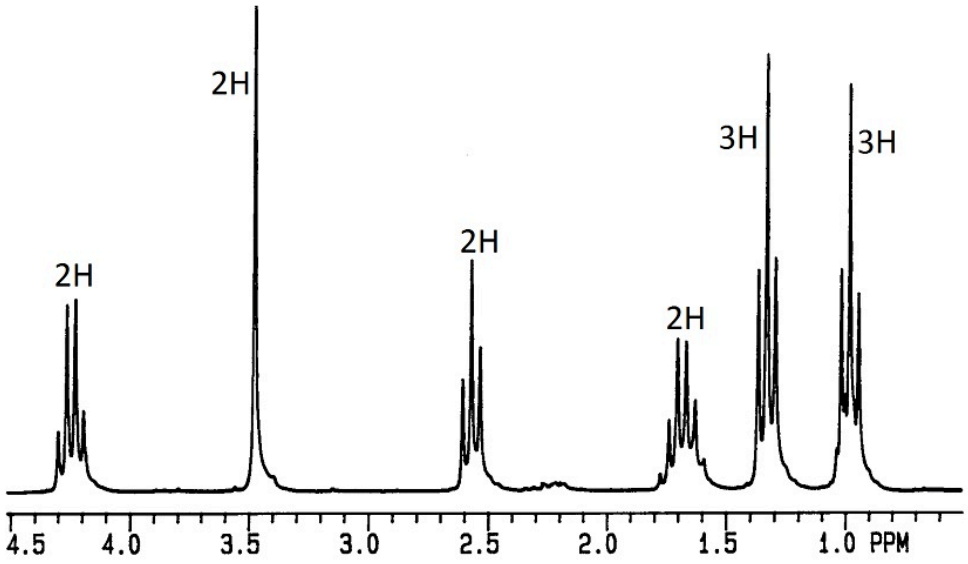




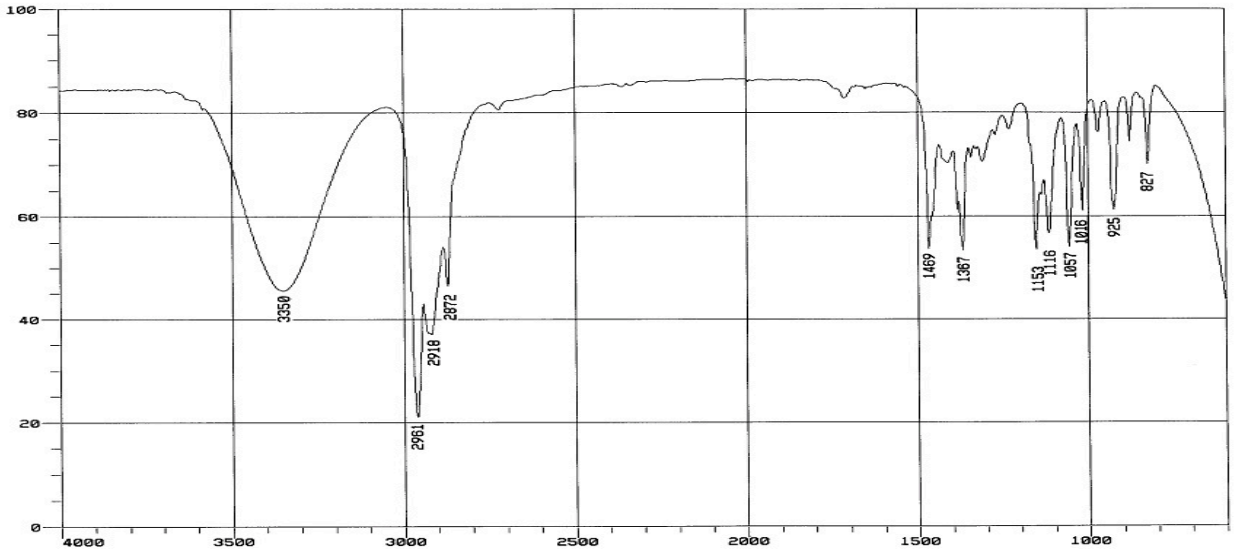

200
180
160
140
120
100
80
60
40
20
0
CDS-01-044
ppm

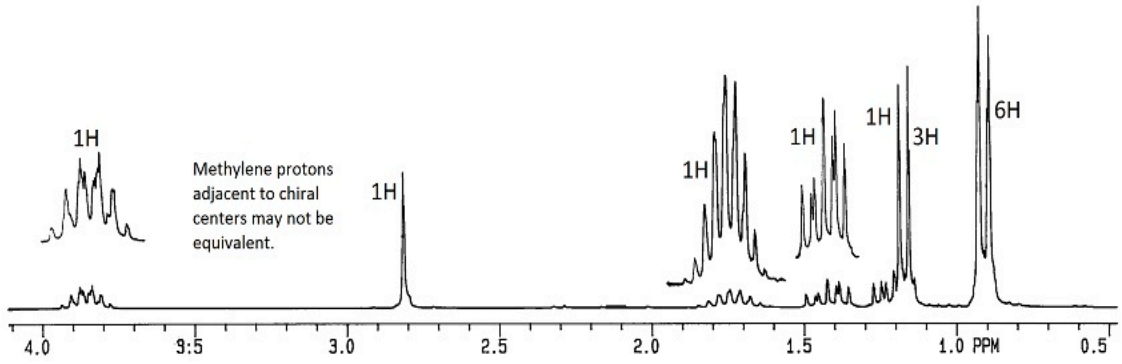
3. Determine the structure of the unknown compound with molecular formula $C_8H_{14}O_3$ using the following spectral data:





4. Determine the structure of the unknown compound with molecular formula $C_6H_{14}O$ using the following spectral data:

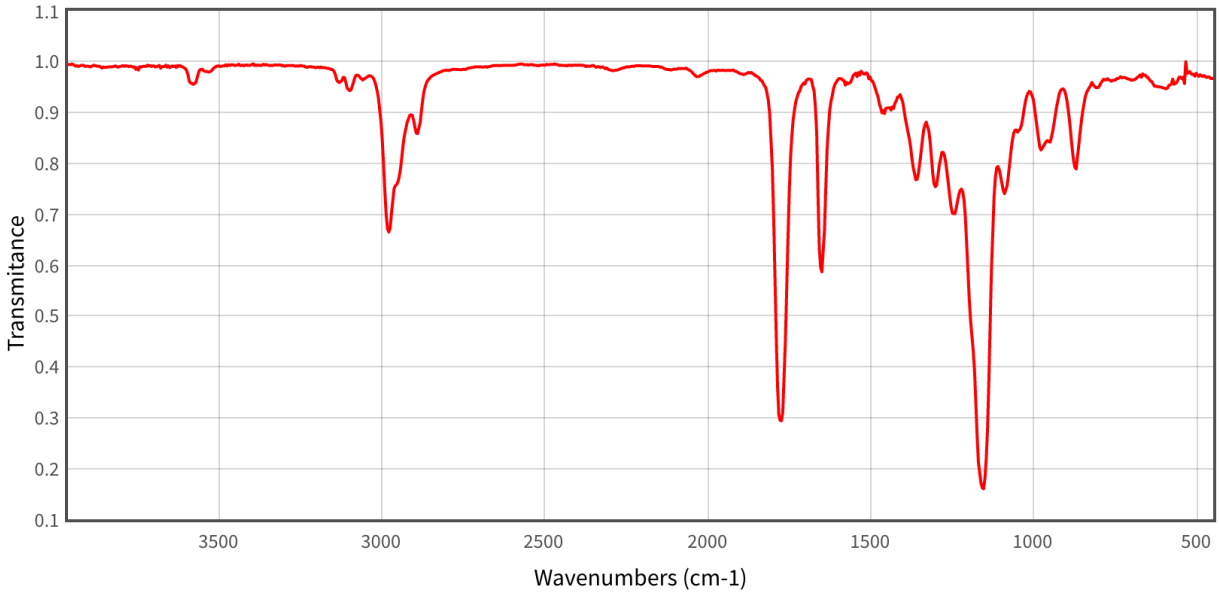


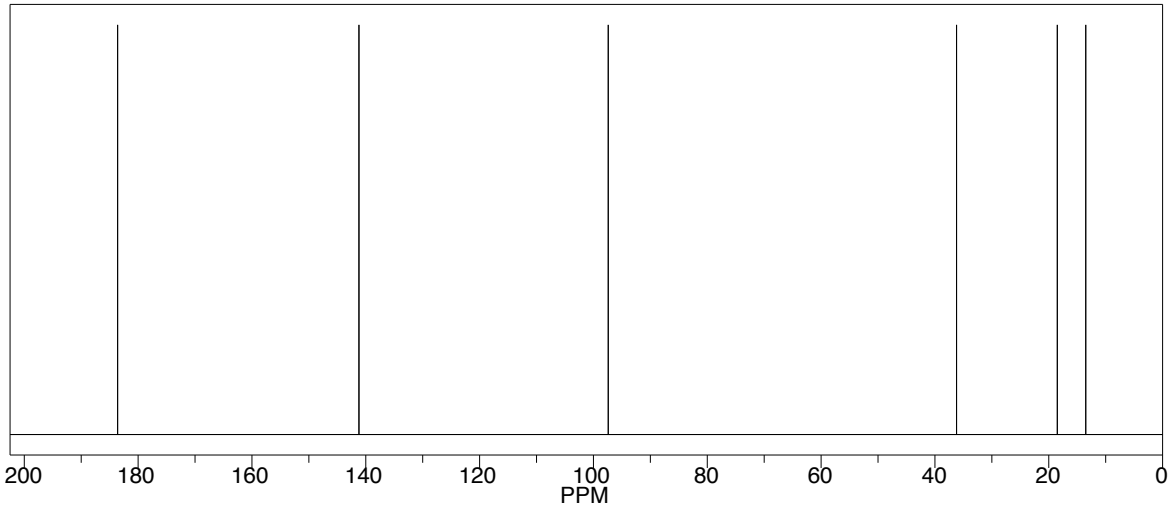


5. For an unknown compound, you are given the following table with the chemical shifts of protons, multiplicity of peaks and integration of each signals. First, sketch a rough ^{1}H NMR spectra based on the information you are given:

ppm	Multiplicity	Integration	Assignment
7.4	dd (doublet of doublets)	1	
4.9	dd	1	
4.6	dd	1	
2.5	t	2	
1.7	m (sextet)	2	
1.0	t	3	

To gain further information, you obtained the following IR and ^{13}C NMR spectra:





In addition, you know that the molecular ion has an *m/z* of 114, and the mass spectrum of the compound shows no isotope pattern for Cl or Br. The degree of unsaturation is 2.

Using comprehensive analysis, come up with the structure for this unknown molecule, and number the protons in your structure. Finally, assign the different hydrogens to their corresponding peaks in the NMR table.

6. Determine the structure of the unknown compound with molecular formula $C_5H_{10}O$ using the following spectral data: