Organic Chemistry I, CHM 3140, Dr. Laurie S. Starkey, Cal Poly Pomona
Nuclear Magnetic Resonance (NMR) Spectroscopy, Part 2 - Chapter 15 (Klein)

^{1}H NMR Problem-Solving Strategies

The goal of solving a ^{1}H NMR spectrum is to determine the structure that is consistent with ALL the NMR data. Since the NMR provides a lot of data, we must develop a systematic approach. First, we must determine what pieces are present. Next, we figure out how those pieces fit together. Finally, we check our structure to see if it matches the spectral data given.

1) If given an IR spectrum: what functional groups (FG) are present? These are pieces to your puzzle.

2) If given molecular formula: check for sites/degrees of unsaturation (DU).
   If saturated, formula fits $C_nH_{2n+2+\#N}$.
   every 2 missing H's = 1 DU
   each DU = a π bond or a ring
   4 DU = a possible benzene ring (3 π bonds, plus 1 ring)

3) Using the peak integration, determine the pieces of your molecule.
   3 H signal = CH_3
   2 H signal = CH_2
   1 H signal = CH or OH or NH

   6 H signal = 2 equivalent CH_3 groups
   4 H signal = 2 CH_2's or a CH_3 + CH (overlapping signals?)

   peaks around 7 ppm = aromatic H's (indicates presence of a benzene ring)
      may be a single peak (singlet) or may be several signals in the region
      a total of 5 H's around 7 ppm = monosubstituted benzene ring
      a total of 4 H's around 7 ppm = disubstituted benzene ring (groups can be *ortho*, *meta* or *para*)

4) Do you have all your pieces? "Add up" your pieces and compare to your molecular formula
   have you accounted for the calculated DU?
   have you accounted for the functional groups in the IR?

5) Put the pieces together! Start with an end piece, such as a methyl (CH_3).
   consider chemical shift
      is it next to an oxygen? (~3.8 ppm)
      is it next to a C=O or a benzene ring? (~2.2 ppm)
   consider splitting patterns (n+1 rule, where n = # of nonequivalent neighbors)
      is it a triplet? It must be attached to a CH_2 (2 neighbors = 3 peaks)
      is it a singlet? There must be no protons on neighboring carbon atoms (0 neighbors = 1 peak).

6) Check your answer! Final structure must match molecular formula, and IR and NMR spectra.
   Look for symmetry. How may peaks should be in the NMR? What would integration be?
   Calculate chemical shifts, predict splitting patterns, and compare to NMR spectrum.

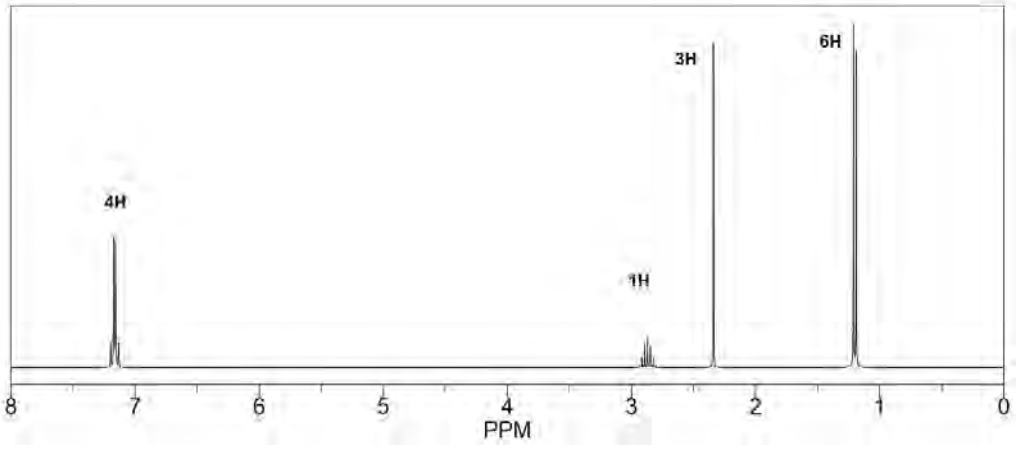
Provide a structure that is consistent with the following ^{1}H NMR data:

$C_9H_{10}O_2$ δ =
7.3 ppm, singlet, 5H
5.1 ppm, singlet, 2H
2.0 ppm, singlet, 3H

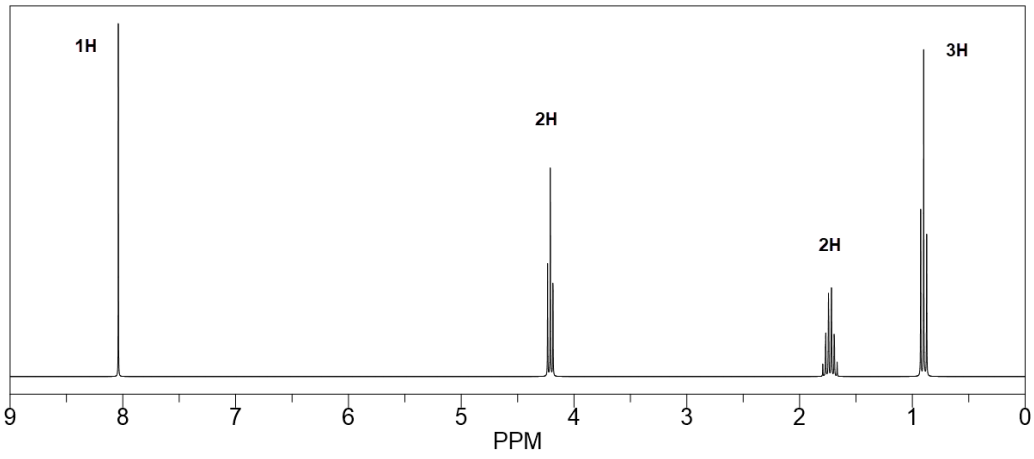
Provide a structure that is consistent with the following ^{1}H NMR data:

$C_9H_{10}O_2$ δ =
7.4 ppm, singlet, 5H
3.6 ppm, singlet, 2H
3.5 ppm, singlet, 3H

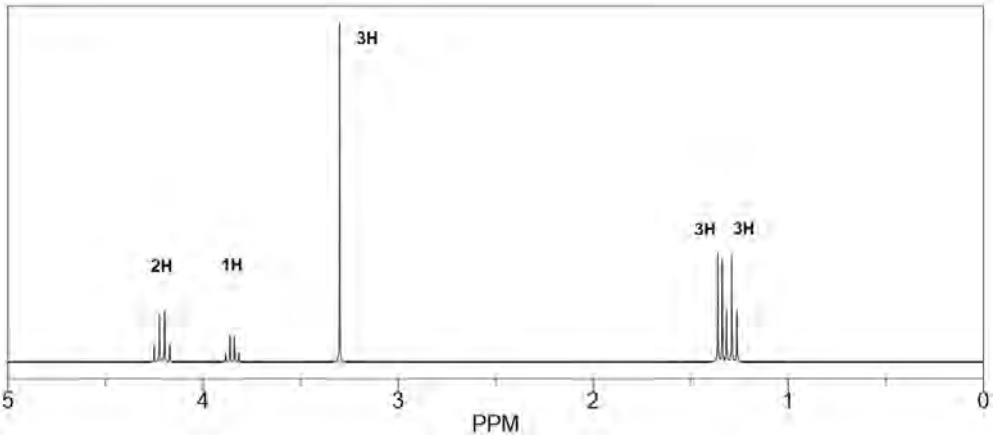
Provide a structure that is consistent with the following ^{1}H NMR data: $C_{10}H_{14}$



Provide a structure that is consistent with the following ^{1}H NMR data: $C_4H_8O_2$



Provide a structure that is consistent with the following ^{1}H NMR data: $C_6H_{12}O_3$



Provide a structure that is consistent with the following ^{1}H NMR data: C_8H_{18}