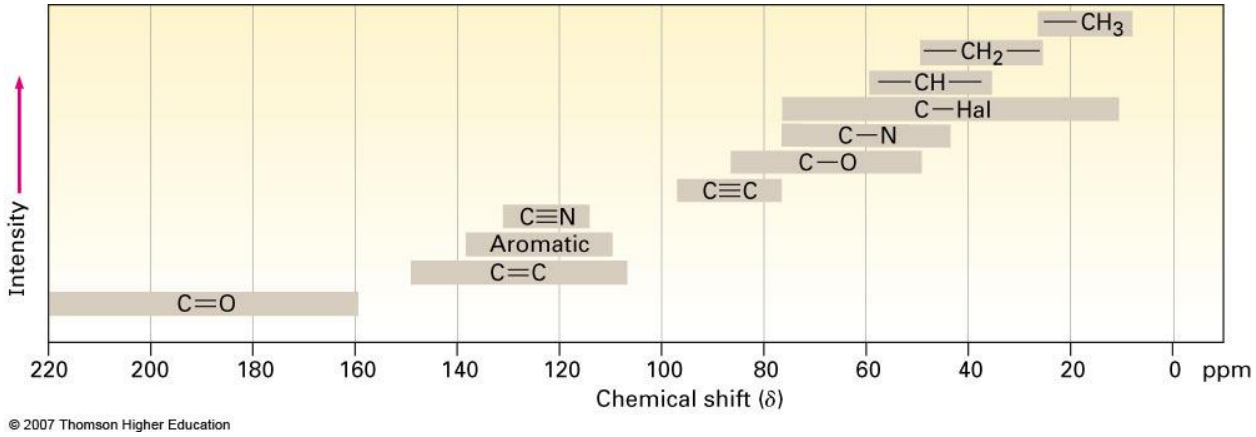
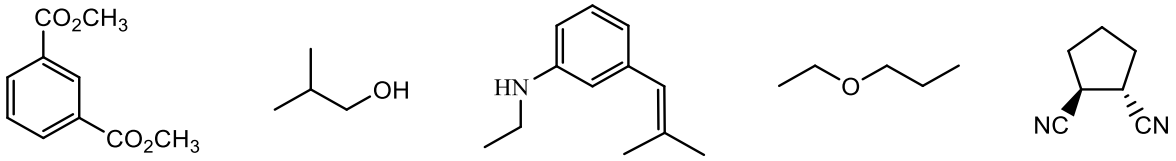
^{13}C NMR SPECTROSCOPY

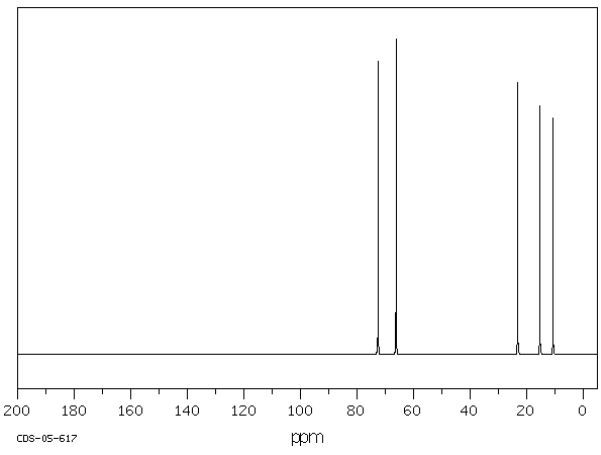


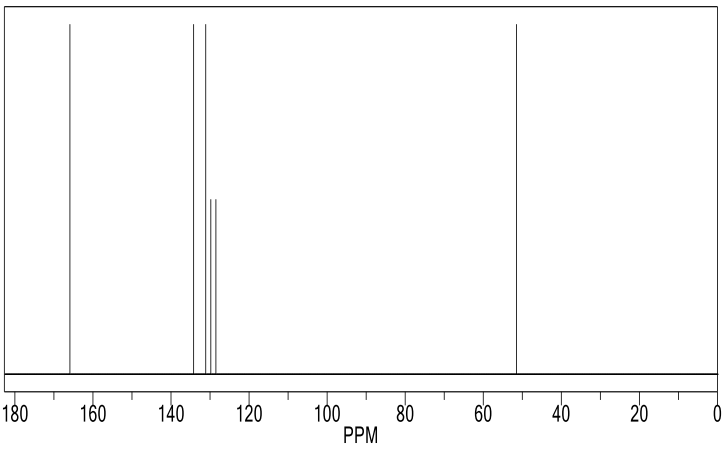
Basics:

To understand the data from Nuclear Magnetic Resonance (NMR) Spectroscopy, you need to understand some basics. First, you must know when two carbon atoms are the same (equivalent) and not the same (inequivalent). Two atoms are considered equivalent only if they are in the exact same environment (i.e. all things around them are identical). Practice by determining how many inequivalent (different) carbon atoms are in each molecule below.



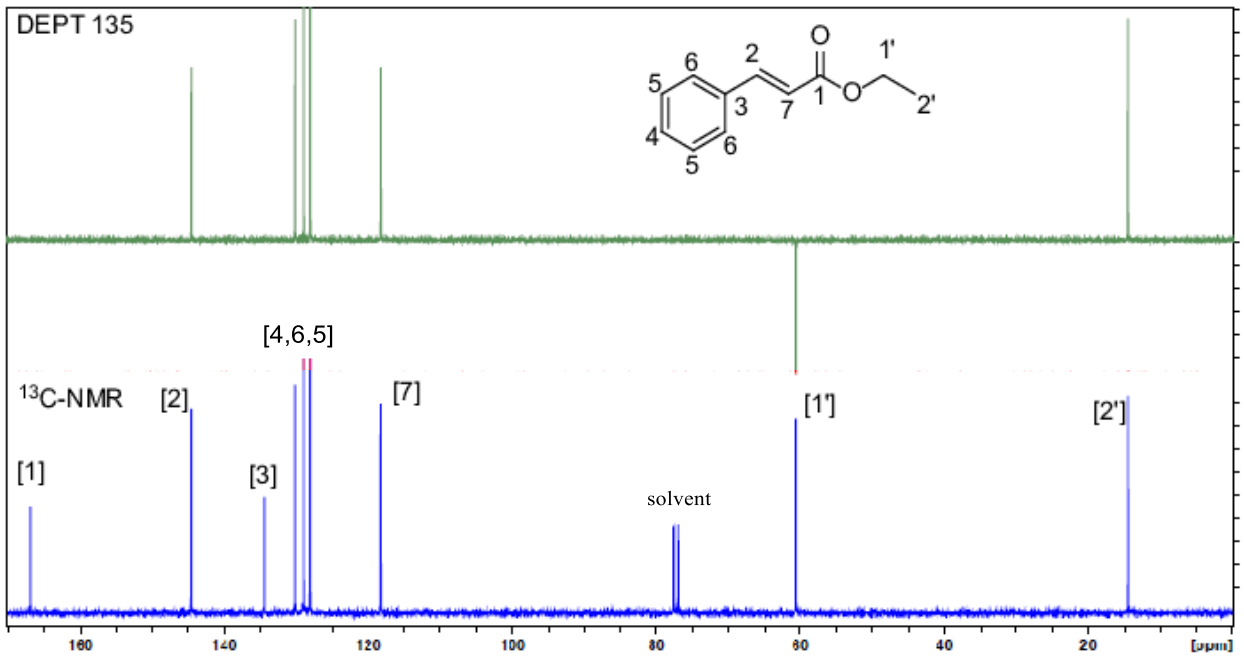
Based on your analysis and using the table above to predict the relative ppm values for the carbons, which of the molecules above could give rise to the following ^{13}C NMR spectra?



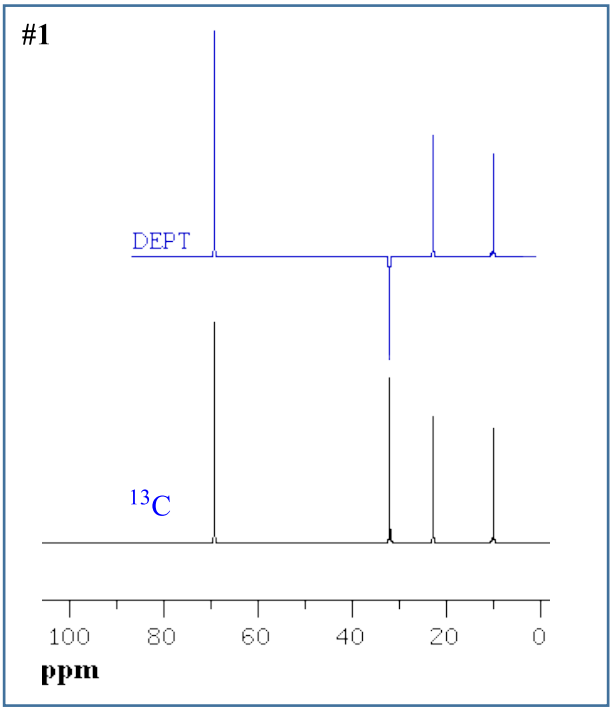


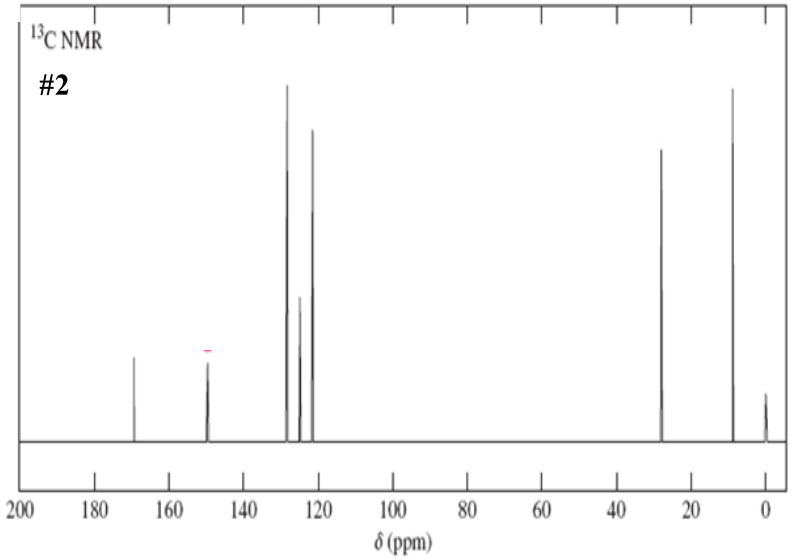
Under ideal conditions, the number of inequivalent carbons is the number of unique signals you would see in a ^{13}C NMR spectrum. Note that sometimes, if carbons are in very similar environments, the signals can accidentally overlap. For example, the ^{13}C NMR spectrum of acetophenone is shown to the right. How many inequivalent carbons do you predict for this molecule? How many peaks do you see in the real NMR?

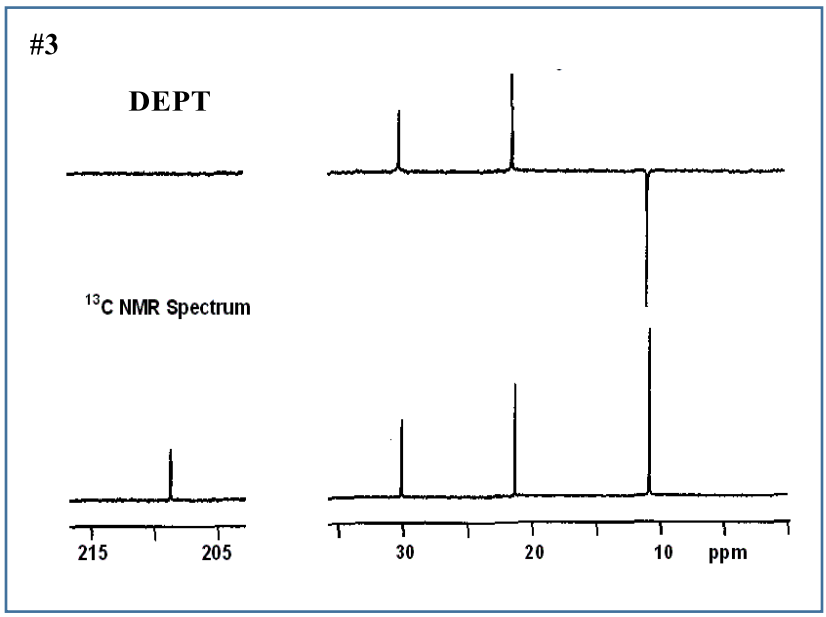
Unlike ^{1}H NMR, in ^{13}C NMR you cannot use peak height to give you the number of carbons in the molecule. You also cannot use splitting patterns to tell about neighboring carbons. Fortunately, there is something called Distortionless Enhancement of Polarization Transfer or DEPT analysis. What this does is modify a standard ^{13}C NMR spectrum to give information about the number of hydrogens attached to each carbon in a molecule. In a DEPT 135 analysis, any carbon that is connected to 2 hydrogens has a signal which points down on the DEPT spectrum (carbon 1' below). Any carbon that is connected to either 1 or 3 hydrogens remains pointing up as it did in the original ^{13}C NMR (carbons 2,2',4,5,6,7). Any carbon that is not connected to any hydrogens at all, disappears from the DEPT spectrum (carbons 1,3). Please remember, DEPT is only useful if you have the ^{13}C NMR for comparison.



Now for some practice. Using the spectra provided (some ^{13}C NMR alone, some with DEPT 135), match the structure with the correct NMR.







Possible compounds: