Summary: Interpretation of NMR Spectra

This ChemActivity is designed to help you remember the important aspects of interpreting NMR spectra. The following is a summary of important points:

**1H NMR**
- **ppm or chemical shift** *(given by location along the x axis)* tells you the amount of electron density around an H. The closer the H is to an electronegative element, the more “deshielded” it is and therefore the higher the ppm number of its peak cluster (farther left on the spectrum). Multiple bonds also cause the signal of nearby H’s to be shifted to the left. Look in the index of your text for “chemical shifts” to find a list of common functional groups with their chemical shifts. Each chemically distinct H should have a unique chemical shift, though in practice different peak clusters sometimes overlap just by coincidence. This can make spectrum interpretation very difficult. Proton NMR peaks usually appear in the 0-10 ppm range.
- **Integration or peak area** *(given by integration line)* tells you the relative size of each peak and therefore the relative number of equivalent H’s represented by each peak. Note that integration only gives you a ratio of peak areas, making it impossible to tell the difference between a 1H to 3H ratio and a 2H to 6H ratio.
- **Multiplicity** is the number of peaks in a peak cluster (also called splitting or proton-proton coupling). It tells you the number of nonequivalent neighbor H’s within three bonds. For example, a doublet (two peaks) tells you there is exactly 1 non-equivalent H within three bonds of the H responsible for this signal. Equivalent H’s don’t split each other.
- **NMR Equivalent Hydrogens** = hydrogens that can be associated via an internal mirror plane or are the same distance away (through bonds AND through space) from every other atom or feature in the molecule. This means that a molecule and it's enantiomer will produce the exact same NMR spectra. (Enantiomers are not distinguishable by NMR!!)

**13C NMR**
- **ppm or chemical shift** in 13C NMR is similar to that of proton NMR. If a C is close to an electronegative element or involved in a multiple bond, or both, you will find the corresponding peak at higher ppm (farther left on the spectrum). Each chemically distinct C should have a unique chemical shift, though in practice different peak clusters sometimes overlap just by coincidence. This can make interpretation of coupled spectra very difficult. This is why decoupled spectra are usually taken. C-13 NMR peaks appear in the 0-220 ppm range, though most peaks are found < 100ppm.
- **Peak area** has LITTLE MEANING in C-13 NMR. Peak area is a function of many things, one being whether the C is 1o, 2o, 3o or 4o. You will not be asked to interpret the meaning of peak area in C-13 NMR.
- **Multiplicity** in a proton coupled 13C NMR spectrum tells you the number of H’s attached to a given carbon. For example, a C that produces a doublet (two peaks) must have exactly 1 H attached to it. Very often chemists record “proton decoupled” 13C NMR spectra. Such spectra have a singlet for each chemically unique carbon. This is useful for complex molecules for which the peak clusters would overlap. A decoupled 13C NMR spectrum tells you the number of different carbon atoms present in the sample.