# Summary of 1H-NMR Interpretation

## I. Number of Signal Sets
## II. "Chemical Shifts" of the Signal Sets

| | |
|---|---|
| 9's (9.0-10.0) | **Aldehyde** $sp^2$ hybridized C-H's |
| 7's (6.5-8.4) | **Aromatic** $sp^2$ hybridized C-H's |
| 5's (4.8-6.8) | **Alkene** $sp^2$ hybridized C-H's |
| 3's (2.8-4.5) | **Oxygenated** or **Halogenated** $sp^3$ hybridized C-H's (halogenated and nitrogenated alkyl C-H's will also come in this window, although no candidates for today's lab). Oxygenated $sp^3$–carbons are routinely present for the following functional groups that contain oxygen single bonds:<br>a. **alcohols**,<br>b. **ethers**, or<br>c. **esters** |
| 2's (1.8-2.8) | **Allylic** $sp^3$ hybridized C-H's ($sp^3$ hybridized C-H's that has a double bond attached to the $sp^3$ hybridized C). Allylic signals routinely appear when one of the following double-bonded functional groups is present:<br>d. **carbonyls**, (ketones, esters, aldehydes, acids, amides)<br>e. **alkenes**, or<br>f. **aromatics** |
| 1's (0.7-2.0) | $sp^3$ hybridized C-H's, with **no attached Functional Groups**<br>g. **Note:** Many molecules with non-functional alkyl portions will give a lot of signal in this area. |
| 0-12 (anywhere!) | **Alcohol/Acid** O-H hydrogens (N-H hydrogens likewise)<br>h. **alcohols**,<br>i. **carboxylic acids** |

1. Check each of the zones. Each one gives you a yes or no answer about the presence of absence of the featured group.
2. End-Check: Check that the functional groups indicated by your chemical shift information match with the structure you believe you actually have! If not, structure needs correction!
3. The regions are somewhat approximate, and have some spillover.
4. For multi-functional complex molecules, there are more complex ways for a C-H to come in some of the above window. For example, an $sp^3$-hybridized C-H with two attached oxygens can come in the 5's, or an $sp^3$-hybridized C-H that is doubly allylic can come in the 3's. In other words, the impact of functional groups is roughly additive.

## III. Integration

These **must be simple whole-number ratios** (2:1, 3:1, 3:2, etc..)

## IV. Splitting

- **N-1 Rule: N lines $\Rightarrow$ N-1 neighbor H's** (H's directly attached to carbons attached to the C-H group causing the signal)
  - The N-1 Rule is useful when working from spectrum to actual structure
- **N+1 Rule: N neighbor H's $\Rightarrow$ N+1 lines**
  - The N+1 Rule is useful when working from structure to actual spectrum

Note: OH hydrogens don't participate in splitting (normally)