

NMR Quick Facts

Chemical shift

- Chemical shift measured in δ (delta) or ppm from TMS (0 ppm)
 - Proton with large shift = *downfield* or *deshielded*
 - Proton with small shift = *upfield* or *shielded*
- Establishes proton's chemical neighborhood
- Golden rule: every chemically unique proton should have unique chemical shift

Integrals

- Area under signal (or signals if proton is coupled to other protons)
- Proportional to #H responsible for signal(s)

Coupling pattern

- Coupling constant (J) measured in Hz
- Establishes #bonds between protons of different chemical shifts
- Magnitude of coupling constant
 - No coupling ($J = 0$ Hz) if protons have same shift
 - Strong coupling ($J = 6-20$ Hz) if protons separated by 2-3 bonds
 - Weak coupling ($J = 0-5$ Hz) if protons separated by >3 bonds
 - If H_A & H_B are coupled, *same* J describes both patterns
- Coupling pattern for proton coupled identically to N neighboring protons
 - Pattern contains $N+1$ peaks
 - Peaks equally spaced (measure J between adjacent peaks)
 - Peak intensity follows binomial coefficients (Pascal's triangle)
 - Singlet (one peak)
 - Doublet (two peaks, 1:1)
 - Triplet (three peaks, 1:2:1)
 - Quartet (four peaks, 1:3:3:1)