

H-NMR: Some Familiar Groups that can become Easy to Recognize

Hydroxyl

1H no splitting => hydroxyl. (Chem shift could be anywhere.)

Aromatics

5H in 7's => mono-substituted benzene

4H in 7's => di-substituted benzene

4H in 7's, with 2 doublets = para di-substituted benzene

Methyl Groups: Clean 3H integral. What's the Methyl Connected to? (each will integrate for 3H)

- 3H singlet in 3's (3-4.5) => oxygenated methyl
- 3H singlet in 2's (1.8-3) => allylic methyl. (Whether allylic to carbonyl, benzene, or alkene)
- 3H triplet in 1's (0.7-2) => CH₃-CH₂
- 3H doublet in 1's (0.7-2) => CH₃-CH

Ethyl Groups: What's the Ethyl Connected To?

Combination of a 3H triplet in the 1's and a CH₂ quartet-or-more in 3's, 2's, or 1's

When an ethyl is connected to a functional group, the CH₂ will be a quartet

- 2H quartet in 3's (3-4.5) => oxygenated ethyl
- 2H quartet in 2's (1.8-3) => allylic ethyl. (Whether allylic to carbonyl, benzene, or alkene)

When an ethyl is NOT connected to a functional group, then the CH₂ must instead be connected to an sp³ carbon that will probably have one or two hydrogens, so:

- The chemical shift of the CH₂ will be in the 1's, and
- 2H sextet in 1's => CH₂CH₂CH₃ (methylene is connected to methyl triplet and a methylene)
- 2H pentet in 1's => CHCH₂CH₃ (methylene is connected to methyl triplet and a methine)

Isopropyl Groups: What's the Methine Connected To? (CH₃)₂CH – something

6H doublet in the 1's combined with a 1H multiplet => isopropyl

Note: the CH must have at least 7 lines (or perhaps more)

- 1H multiplet in 3's (3-4.5) => oxygenated isopropyl
- 1H multiplet in 2's (1.8-3) => allylic isopropyl. (Whether allylic to carbonyl, benzene, or alkene)
- 1H multiplet in 1's => isopropyl must be connected to an sp³ carbon

Propyl:

CH₃CH₂CH₂-something

Will always have: 3H triplet 1's and 2H sextet 1's and a CH₂ somewhere:

If the propyl is connected to a functional group, then there will be a CH₂ pentet:

- 2H triplet in 3's (3-4.5) => oxygenated propyl (plus CH₂ sextet in 1's and CH₃ quartet in 1's)
- 2H quartet in 2's (1.8-3) => allylic propyl. (Whether allylic to carbonyl, benzene, or alkene)