Welcome everyone!

Today's Experiment
NMR Analysis

We will begin at 12:10pm.

Please add your group number to the beginning of your name.

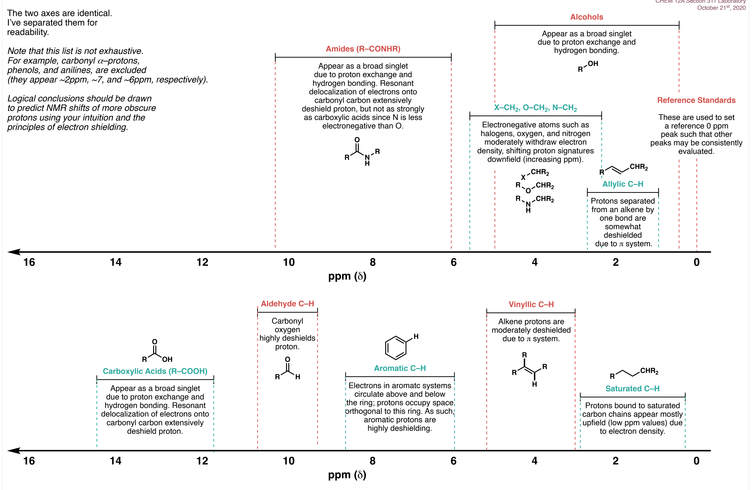
Use this time to ask questions and chat!

Common Functional Group Proton NMR Shifts

The two axes are identical. I've separated them for readability.

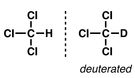
Note that this list is not exhaustive. For example, carbonyl α–protons, phenols, and anilines, are excluded (they appear ~2ppm, ~7, and ~6ppm, respectively).

Logical conclusions should be drawn to predict NMR shifts of more obscure protons using your intuition and the principles of electron shielding.



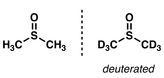
Common Solvent Residual Peaks

Chloroform

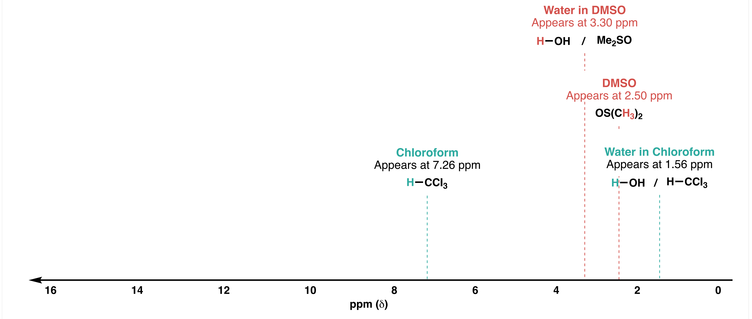


deuterated

Dimethyl Sulfoxide (DMSO)



deuterated



Stepwise NMR Spectra Processing

1. Set CHEM 12A Template Defaults
Open the file available on bCourses entitled "Chem 12A MNova layout template".

2. Open Sample FID (Free Induction Decay)
Open the FID file provided for the given sample.

3. Apply Processing Corrections
Select the Processing tab on the top of the page in MNova.
Click on "Auto Baseline Correction" and "Auto Phase Correction".

4. Select a Reference Peak
Press "R" on your keyboard and select the reference peak (usually near 0 ppm).
Reassign this peak to 0.00 ppm.

5. Integrate Each Peak
Press "I" on your keyboard and click and drag over each peak. Note that the first peak you integrate will automatically normalize to 1.00.

6. Normalize Integrals
Select an peak of known proticity (proton count) and right click it's integration value. Select "edit integral" and reassign its normalized value to the known proton count.

7. Pick through peaks
Press "command K" on OS X or "control K" on Windows and pick through each peak.

8. Zoom in on spectrum and export
Press "Z" once to highlight across an entire horizontal region. Zoom in from the leftmost peak to the rightmost peak. Press "Z" again to highlight across an entire vertical region. Zoom in from the tip of the largest peak to just below the baseline.

You are now ready to export the document as a **PDF** for submission.

Compound Ratios for NMR Integrals

This is an example from the prelab.