NMR spectroscopy in non deuterated solvents.

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The acquisition of NMR spectra in non deuterated solvents is not very different from regular acquisitions in deuterated solvents. The most noticeable difference is that you won't be able to lock the magnet or to shim as usual by looking at the lock signal's strength.

After placing your sample in the magnet, loading appropriate parameters, and selecting the solvent (choose from the list the deuterated solvent equivalent to your protonated solvent) load the shims as usual with `setlock`. This macro also sets Z0 (the magnetic field's strength) to a value appropriate to your solvent. Notice that the [Find Z0] button will not work as it relies on the presence of a deuterated solvent. Then turn the lock off in the Start, Lock parameter panel. To shim using the signal of your protonated solvent, first make sure the probe is tuned to detect protons, then select from the main menu: Acquisition > Do Gradient Shimming > Use 1H/gradient map. This procedure works best with solvents that produce only one major peak. With other solvents, like THF, it may not be completely successful, but repeating the shimming process a second or third time can help. If the resulting spectrum is unacceptable, or if your solvent doesn't have any hydrogen atoms, follow the instructions in the writeup "*Gradient shimming non deuterated solvents*" available in our web site. If your solvent does not have any hydrogen atoms, the only way to shim is by monitoring the shape of a signal in your spectrum.

In the case of proton NMR in solvents containing hydrogen atoms, the solvent's signal can be too strong for the receiver, even at `gain=0` and you may get an error message similar to "Receiver overflow, reduce pulse width". If this happens just do as you are told and reduce the pulse width (set `pw=1`) and try again. If your sample is sufficiently concentrated, you may get an acceptable spectrum despite the very large solvent peak(s). Notice that close to the base of your solvent peaks some signals may appear that look like spinning side bands; i.e. they are symmetrical around the main peak. However, they appear at frequencies that do not correspond to the spinning rate or even the proton-carbon coupling constant and they are usually out of phase. They arise from an unbalanced spinner (due to user abuse). Changing the spinner or turning the spinning off will eliminate these artifacts. Please don't drop the spinners!

If your sample is dilute or if you have a very large solvent peak, your spectrum will look "noisy". In this case, further accumulation of scans will not help. The problem is not of poor signal to noise but of limited dynamic range: your weak signal is poorly digitized when a very strong signal is present. The best course of action is to eliminate the offending peaks using a solvent suppression technique. The easiest technique is *presaturation*. It gives acceptable suppression in most cases, but when a more effective and selective method is required, or when you need to suppress multiple peaks as is the case with THF, the best method is *wet1D*. This is a more sophisticated pulse sequence that employs shaped pulses and magnetic field gradients to perform the suppression. Both wet1D and presaturation are explained in a separate application note.