NMR Experiments Guide:

Ideally your samples should be >10 mg /600uL of solvent (or 20mMol). For more dilute samples you should run more scans. When running long overnight experiments its best to select (check) the TUNE option to increase the sensitivity of the spectrometer. Approximate experimental times are posted. You may decrease the number of scans or increase them depending on the concentration of your sample. For overnight experiments with 2D and 13C NMR make your sample as concentrated as you can without compromising too much on sample volume so that you experiment doesn't error (for example, your sample loses lock or is unable to lock). Thoughtful sample preparation and experimental planning is the key to successful NMR data acquisition.

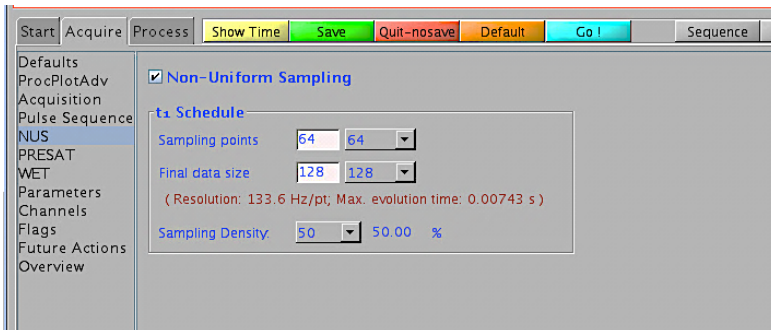
For 2D experiments: ***Acquire> Default*** Tab

Experiment		**Scans per t1 increments**	**T1 increments**
gCOSY	$^{1}J_{H\text{-}H}$	4	>200 Exp time ~10 mins
ASAPHMQC	$^{1}J_{H\text{-}C13}$	16 or more	>200 Exp time ~15 mins
gHMQC/ gHSQC	$^{1}J_{H\text{-}C13}$	16 or more	>256 Exp time ~ 2 hr, 40 mins
gHMBC	$^{2\text{-}3}J_{H\text{-}C13}$	16 or more	>256 Exp time ~ 2 hr, 40 mins
NOESY	Start with default settings but set mix time =500-700ms		

Note: ASAPHMQC gives the same results as the gHMQC or gHSQC in much shorter times.

Another way to maximize your NMR time is to use **NUS** (non-uniform sampling) an option **to decrease the run time** of your experiments with more scans. If an experiment has NUS capabilities, after you double click on the experiment in the **studyQ**, you will see the NUS tab in the acquire option: ***Acquire> NUS***. Go to the NUS tab and check the non-uniform sampling option (see figure below). If the NUS tab is missing that particular experiment does not have this option.

Experiment		**Scans per t1 increments**	**T1 increments**
ASAPHMQC	$^{1}J_{H\text{-}C13}$	16 or more	>200 Exp time ~ 7 mins
gHMQC/ gHSQC	$^{1}J_{H\text{-}C13}$	16 or more	>256 Exp time ~ 1 hr, 21 mins
gHMBC	$^{2\text{-}3}J_{H\text{-}C13}$	16 or more	>256 Exp time ~ 1 hr, 24 mins



- Make sure your T1 increments >128. For dilute samples (set >200).
- Sampling density must be 50% or more.

When you use NUS, you should make sure the version of MNOVA you're using is 10.0.2.

Tip for 13C NMR:

The key to getting a quick carbon is getting the greatest number of scans in the shortest amount of time to increase your signal to noise ratio. This can be done by lowering the acquisition time. The current **default acquisition time for Carbons is 1.049 seconds which is WAY longer than necessary for small molecules**. To change your acquisition time, double click on your CARBON in the studyQ. In the ***Acquire>Acquisition*** tab, change the Acquisition time to desired value (no less than 0.25s) then change the number of scans. MAKE SURE THAT YOUR ACQUISITION TIME IS NOT TOO LOW OR YOU WILL *CLIP OFF* PART OF YOUR FID AND INTRODUCE ARTEFACTS IN YOUR SPECTRUM. If you're unsure run a 15 min CARBON and check your FID to make sure it is not truncated.

Reem: "The lowest **acquisition time** I've been able to use is **250 ms** (make sure you change the units to ms from seconds). This specific acquisition time allows you to **increase the number of scans to 680 scans** which is more than four times what you can fit into a normal 15min time slot. This is usually enough scans to get a decent carbon on **samples as little as 2-3 mg** depending on the MWT. It at least gives you a good idea of whether you really need overnight time. Also, another useful tidbit of information is: **you have to SQUARE the number of scans to DOUBLE the height of your peak.** This gives you a good estimation of how long you need to run your sample."

To reload the shim file type in command line: **rts('last') su** and hit return.