

# NMR Parameter Test

Name: \_\_\_\_\_

Date: \_\_\_\_\_

NetID/  
NOT UIN \_\_\_\_\_

PI: \_\_\_\_\_

This test is designed to ascertain whether you understand some of the common parameters in NMR. Successfully passing this test will make more parameters available to you in automation. Show your work on a separate sheet of paper, write out your answers legibly, put your name on every sheet, and good luck.

1. Due to an inter-lab prank a bottle of good chloroform-d was contaminated with non-deuterated chloroform, which was used to make a sample destined for a journal that requires the target material to have the largest signal in the proton spectrum. The sample was actually prepared in 98.6% chloroform-d, which has a density of 1.5 g/mL and molecular weight of 120.38 g/mol. What is the concentration in millimolar of non-deuterated solvent?
2. Suppose the sample in question 1 has a non-deuterated solvent concentration of 74 mM. What is the minimum concentration for the sample's target material assuming: 1- everything relaxes at the same rate, 2- the target's largest spin concentration comes from a single methylene group that produces a single signal split 1:3:3:1, and 3- that the resulting  $^1\text{H}$  signal from the solvent is a singlet.
3. When doing a  $T_1$  experiment on a target compound, a zero crossing of 18 seconds was found. Given that the zero crossing is equal to  $T_1 \ln(2)$ , how long should the relaxation delay ( $d_1$ ) be if the acquisition time ( $aq$ ) is 6 seconds and you want to recover 99% of the magnetization between scans using a  $90^\circ$  pulse? Suppose the target signal is a singlet and well-separated from any others and has a full width at half height (FWHH) of 2.4 Hz, what would the minimum integration width be (in Hertz) for a 99% quantitative integral?
4. When running a carbon with an (initial) acquisition time ( $aq$ ) of 1.38 seconds on a Bruker instrument you decide to change your spectral width ( $sw$ ) from 235 ppm to 325 ppm. Without further adjustment, what is the new acquisition time? If the transmitter offset frequency ( $\nu_{1p}$ ) is set to 75 ppm, what is the frequency range acquired (in ppm)?
5. Expect questions of common conditions in NMR and how you can use the basic NMR parameters and experiments to address them.
6. Expect questions that address sample viability for NMR and what to do about it if the sample isn't amenable to NMR analysis.