PROBLEM SET 2, BCMB 8190

1) The width of a Lorenzian line in an NMR spectrum is 2 Hz. If this line width is totally dictated by spin relaxation, what is the T_2 for the site? If one Hz of the line width is contributed by magnet inhomogeniety, what are T_2^* and T_2? If we multiplied the FID from the last case by an exponential with decay constant of 1s before Fourier transformation, what is the line width?

2) You are going to acquire a signal averaged ^{13}C spectrum of a compound with a 5 sec T_1 and 0.3 sec T_2* for most carbons. You anticipate resonances over a 200 ppm region at 50 MHz (50 MHz for ^{13}C). What values for the following acquisition and processing parameters would you choose in order to optimize signal to noise while maintaining acceptable resolution:

a) acquisition time
b) number of time domain points
c) pulse angle
d) delay between acquisitions
e) line broadening (exponential multiplication for a weighting function)

3) If our S/N in a 4 min acquisition is 5:1. What would the S/N be after a 100 min acquisition?

4) Couplings between 5' and 5'' protons and the phosphate phosphorus in a 5' nucleotide are observed to be 6.0 and 8.0 Hz, respectively. Using the following formula

$$J_{P,H} = 21 \text{ x } \cos(\theta)^2 - 2.25$$

and assuming idealized rotomer geometries about the C5 - O5 bond, calculate the rotamer populations for this molecule.

5) The ^{13}C-^{15}N coupling constant between the amide nitrogen and its carbonyl carbon (C') in a polypeptide is 15 Hz. What would you expect the coupling constant for a Cα carbon and the directly bonded nitrogen to be? How would you expect the C'-N coupling compare to the C-C coupling in ethylene?