BCMB 8190
PROBLEM SET 4 - ANSWERS

1)

NOE => $\omega_c \tau_c << 1$

$$\tau_c = \frac{1}{T_1} \frac{r^6}{\gamma_H^2 \gamma_C^2 \hbar^2} =$$

$$= \frac{1}{30\times10^{-3}} \frac{(1.1\times10^{-18})^6 (1.05\times10^{-27})^{-2}}{(2.7\times10^4)^2 (2.7\times10^4 \times .25)^2}$$

$$\tau_c = 1.6 \times 10^{-9}\ s$$

Using Stokes-Einstein,

$\eta = 0.01$ poise $= 10^{-3}$ Pa.s

$$\tau_c = \frac{4\pi\eta a^3}{3kT}$$

$a = 9.3 \times 10^{-8}$ cm.

a small protein.

2)

Assuming adenine H2s have the six-membered ring of other adenines 3A above and below,
each would shift the H2 upfield by 0.75 ppm. Hence, a flipped out base would have an H2 resonance downfield by 1.5 ppm.

3)

According to Spera and Bax the alpha carbon resonance of an amino acid in an alpha helix would be about 5 ppm downfield of its corresponding position in a beta sheet.