

# CHEM/BCMB 819D

## Final Exam. Answers

12/16/02

I.

1. 5.5 Hz
2.  $>1035, <1042$
3.  $\approx 300$  pts
4. 125 Hz
5.  $6 \times 10^7$
6. 167 Hz
7. above
8. 60 Hz
9.  $90^\circ$
10. proton
11.  $\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$
12. 129 MHz
13.  $\alpha$  helix
14. A-U, G-C
15. NOESY, H<sub>g</sub>
16. 2.7, 3.3, 5.0
17. J, dipolar coop. chem shift ...
18. NH<sub>4</sub><sup>+</sup>
19. Mn<sup>2+</sup> T<sub>1,2</sub> shorten
20. 12.8 Hz

- II
1. 44.4 ppm - glycine
  2. i-1, alanine
  3. IAG, FAG
  4. HCCH TOCSY
  5.  $\alpha$  helix

III.

$$a. I_{z1} \xrightarrow{90_y} I_{x1} \xrightarrow{J} 2I_{1y}I_{z2} \xrightarrow{90_y} 2I_{1y}I_{zX}$$

$$\xrightarrow{90_y} -I_{1y}I_{zZ}$$

$$I_{z3} \xrightarrow{90_y} I_{x3} \xrightarrow{J} I_{x3} \xrightarrow{90_y} -I_{z3} \xrightarrow{90_y} -I_{x3}$$

note: these are opposite signs -  
sequence on midterm gave like signs

$$b. +2I_{1z}I_{2y} + -I_{x3}$$

subtract. them.

c. zero + 2Q coherence, single quantum

$$d. G1 = \pm \frac{1}{2} G2$$

IV.

a)  $d_{H1-H4'} = 2.7 \text{ \AA}$

$$d_{H1-H3'} = \sqrt[6]{\frac{4}{7}} \times 2.7 = 3.4$$

b)  $2.0 = 5.7 \cos^2 \varphi - 0.6 \cos \varphi + 0.5$

$$\varphi = \pm 55, \pm 118$$

+60 is most likely

c)  $H_{4'}$ ,  $H_{3'}$  equidistant  $\Rightarrow$

$\varphi$  closer to zero,  $+30^\circ$  ?..

d)

$$J = 5.7 \cos^2 \varphi - 0.6 \varphi + 0.5$$

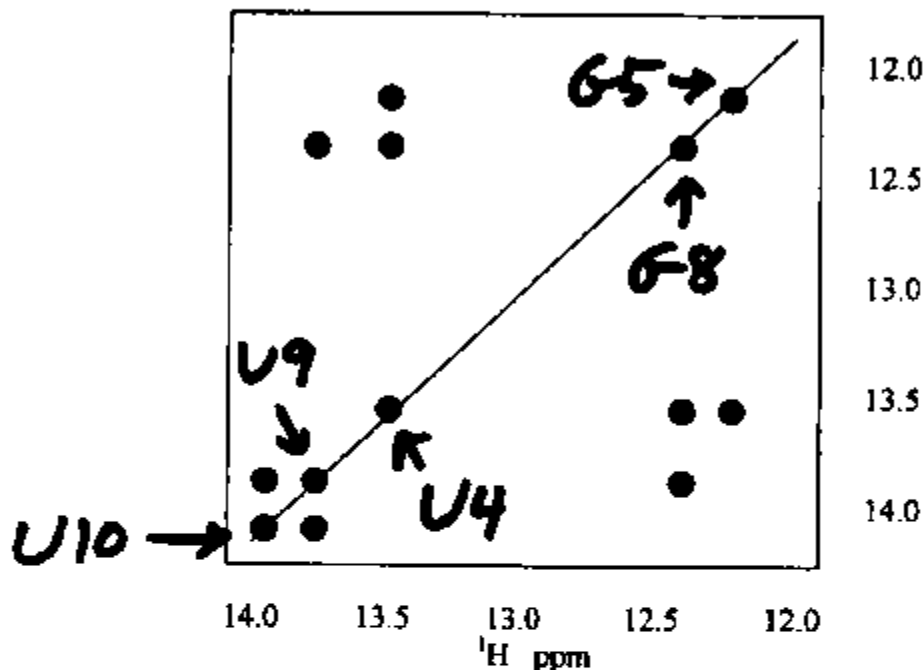
$$\varphi = 30 \Rightarrow J = 4.3 \text{ Hz}$$

e) lines are too broad to measure coupling.

Part 5 (30 pts)

(6 pts each assignment)

The following represents the imino portion of a  $^1\text{H}$ - $^1\text{H}$  NOESY on the following RNA molecule that dimerizes to form an A form helix: AACUGCAGUU. Numbering the bases from left to right starting at 1, give a probable assignment for the resonances occurring on the diagonal. How would information from a  $^{15}\text{N}$ - $^1\text{H}$  HSQC help?



1	2	3	4	5	6	7	8	9	10
A	A	C	U	G	C	A	G	U	U
U	U	G	A	C	G	U	C	A	A
10	9	8	7	6	5	4	3	2	1