

BCMB 8190
PROBLEM SET 7 - ANSWERS

1)

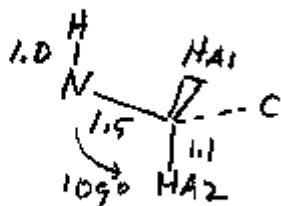
• Volumes are proportional to Vr^6
in short τ_{ms} isolated spin pair approx.

using HA_1-HA_2 as a reference.

$$r_{NH-HA_1} = \sqrt[6]{28/1.6} \cdot 1.75 = 2.82$$

$$r_{NH-HA_2} = \sqrt[6]{28/0.5} \cdot 1.75 = 3.42$$

max separation of $NH + HA_2$ is at
 $\phi \approx 120^\circ$. ie. in this case.



$$NH-HA_2 = 3.04$$

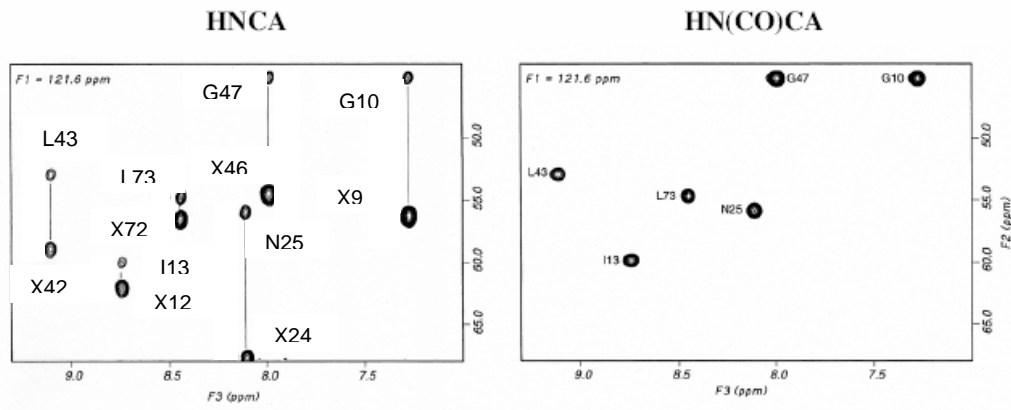
$$NH-HA_1 = 2.66$$

These are as close as we get to
observed NOE.

- 2)
- a) 3 dimensions
 - b) $t_1 - 15N$, $t_2 - 1H$, $t_3 - 1H$
 - c) magnetization proportional to an NOE
 - d) HMQC-NOESY

3)

a)



b) Upfield peaks are weaker because the two bond Ni to Ci-1 coupling constant is smaller

c) Weaker peaks will not always be upfield – it is coincidence in this case. They just occur at the carbon chemical shifts of the respective alpha carbons.