

# CS 663: Algorithms in Structural Molecular Biology

## Assignment #5

Please submit to your TA by Due Date

### HSQC, NOESY and TOCSY

Below is a table for a hypothetical protein which has been assigned the following chemical shifts. <sup>1</sup>

1. Plot the <sup>15</sup>N/<sup>1</sup>H HSQC spectrum showing the resonances for the residues  $r_1$  to  $r_{11}$ . The <sup>15</sup>N chemical shifts are plotted on the Y-axis, and <sup>1</sup>H chemical shifts are plotted on the X-axis, but increasing from right to left.
2. Plot in the strip mode the <sup>15</sup>N-TOCSY-HSQC spectra for residues  $r_1$  to  $r_5$ .
3. By looking at the side-chain hydrogens and their chemical shifts, can you guess the identity of the 11 amino acids? Note you may have multiple answers for one residue.
4. Assume that the given residues form an alpha helix. Using the information in chapter 8 of the book, plot the 2D NOESY spectrum showing the peaks for residues  $r_1$  to  $r_{11}$ .
5. Now using only the NOESY spectrum you constructed, draw the NOESY Interaction Graph.

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<sup>1</sup>Thanks to Dr. Pei Zhou for providing data and comments for preparation of this assignment.

	N	HN	$H_\alpha$	$H_\beta$	$H_\gamma$	$H_\delta$	$H_{\delta'}$	$H_\epsilon$
$r_1$	122.2	8.45	4.08	1.61,1.87	1.35,1.67	2.95,3.05		
$r_2$	122.2	7.64	4.08	1.76,1.31	1.47,1.55	1.66		2.91
$r_3$	120.9	7.33	4.18	1.46,1.80	1.64	0.73	0.87	
$r_4$	110	8.5	3.98,3.73					
$r_5$	123.6	7.89	4.13	1.27				
$r_6$	121.5	7.28	4.89	2.78,3.22				
$r_7$	120.9	7.28	4.23	2.85				
$r_8$	122.2	9.16	4.23	2.61,3.04				
$r_9$	121.5	6.93	4.39	1.65,1.85	1.45	1.11	0.88	
$r_{10}$	131	9.47	5.55	1.73,1.85	1.39,1.48	1.61		2.86
$r_{11}$	126.3	9.31	5.55	1.07,1.60	1.48	0.28	0.88	