CS 196: Algorithms in Drug Design
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. [1]

1. Plot the ^{15}N/^{1}H HSQC spectrum showing the resonances for the residues r_1 to r_{11}. The ^{15}N chemical shifts are plotted on the Y-axis, and ^{1}H chemical shifts are plotted on the X-axis, but increasing from right to left.

2. Plot in the strip mode the ^{15}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.

[1] Thanks to Dr. Pei Zhou for providing data and comments for preparation of this assignment.

	N	HN	H_α	H_β	H_γ	H_δ	$H_{\delta'}$	H_ϵ
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	