AMS Common Exam Part B, Computational Biology Track, June Exam 2009

Name: _____ **ID Num:** _____

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DO THREE OUT OF FOUR QUESTIONS ONLY: Questions are based on AMS-535 (Questions 1-2) and CSE-549 (Questions 3-4). Each question is worth 25 points.

Question 1: If the association of a ligand L with receptor R in the condensed phase (water) is defined as the *absolute* experimental binding free energy (ΔG_{exptl}), clearly draw the thermodynamic cycle which can be used to computationally estimate the *absolute* binding free energy (ΔG_{calcd}).

Neatly write the simple expression which relates how all legs of the cycle are equivalent to ΔG_{expt} and ΔG_{calcd}. Which term best corresponds to the hydration free energy of the ligand?

Question 2:

For the 20 naturally occurring amino acids fill in the following table. Indicate which of the folloing properties best-describes each amino acid. Properties = hydrophobic, hydrophilic, aromatic ring, 5-membered ring negatively charged, positively charged, ring in protein backbone, disulphide bonds, smallest side chain.

	Name	3 letter code	1 letter code	Property
01				
02				
03				
04				
05				
06				
07				
08				
09				
10				
11				
12				
13				
14				
15				
16				
17				
18				
19				
20				

Question 3: Sequencing By Hybridization. Given is the set S below, representing all 3-mers from an unknown string s. Find the string s such that

Spectrum(s, 3) = {ATG, GGG, GGT, GTA, GTG, TAT, TGG}

(a) By using the Hamiltonian path approach. Label edges and vertices of the graph and give all possible sequences s satisfying the above condition. Does this path visit every edge of the constructed graph exactly once?

(b) By using the Eulerian path approach. Label edges and vertices of the graph and give all possible sequences s satisfying the above condition. Does this path visit every vertex of the constructed graph exactly once?

Question 4: Spectral Convolution. Given are the two sets A and B below, representing two spectra. Compute the similarity value between A and B by using spectral convolution.

A = {11, 17, 31, 33, 41}, B = {11, 20, 34, 40, 48}

Assume that there are two mutations and explicitate the computation of the value that you have obtained.