AMS Common Exam Part B, Computational Biology Track, May Exam 2011

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: Note this question has multiple parts

(1a) Write the most common functional form (i.e. the specific equations) for the classical potential energy functions used in computer simulations that employ a Molecular Mechanics force field. Explicitly label all variables and constants.

(1b) Draw a thermodynamic cycle commonly used to determine the *relative* free energy of binding ($\Delta\Delta G_b$) between two ligands A and B with a protein receptor P. Clearly label all parts and terms of your figure.

Write the simple expression which shows how two legs of the cycle (computed using techniques such as free energy perturbation) are equivalent to the difference in the experimental binding energies ΔG_b (A) and ΔG_b (B) between the two ligands.

Which term most closely corresponds to the *relative* free energy of hydration between ligands A and B?

Describe how the *absolute* free energy of hydration for ligand A (or B) might be estimated?

Question 2: Note this question has multiple parts

(2a) List the 1 and 3 letter codes of all 20 amino acids.

01:	11:
02:	12:
03:	13:
04:	14:
05:	15:
06:	16:
07:	17:
08:	18:
09:	19:
10:	20:

(2b) Indicate which two residues are negatively charged under most conditions.

(2c) Indicate which two residues are positively charged under most conditions.

(2d) Which residue can form disulfide bonds?

(2e) Which residue is incorporated into the protein backbone?

(2f) Which two residues incorporate a "benzene" ring into the side chain?

(2g) Which three residues have "hydroxyl" groups?

(2h) Which charged residue has a planer "guanidinium" group?

(2i) Which residue has a fused two-ring side-chain?

(2j) Which residue has the smallest side-chain?

(2k) List four functional groups on protein side-chains or the backbone capable of H-bonding.

Question 3: Suppose you are given three strings of characters: X, Y, and Z, where $|X| = n$, $|Y|=m$, and $|Z|=n+m$. Z is said to be a shuffle of X and Y iff Z can be formed by interleaving the characters from X and Y in a way that maintains the left-to-right ordering of the characters from each string.

(3a) Show that cchocohilaptes is a shuffle of chocolate and chips, but chocochilatspe is not.

(3b) Give an efficient dynamic-programming algorithm that determines whether Z is a shuffle of X and Y. Hint: the values of the dynamic programming matrix you construct should be Boolean, not numeric.

Question 4: Briefly describe how new generation sequencing technologies compare to traditional Sanger sequencing.

What types of experiments are possible with new generation technologies which were not with older technologies?