

AMS Common Exam Part B, Computational Biology Track, June Exam 2007

DO THREE OUT OF FOUR QUESTIONS ONLY.

One question must be based on AMS 535 (questions 1-2) and one question must be based on CSE 549 (questions 3-4). The remaining question can be from either section.

Name: _____

Question based on AMS 535:

1. Draw the thermodynamic cycle commonly used in techniques such as MM-GBSA and MM-PBSA to compute the absolute free energy of binding (ΔG_{bind}) between a ligand L and receptor R. Clearly label all parts of your figure. If the association of L with R in water is defined as the experimental binding free energy (ΔG_{expt}) write the simple expression which relates how the other legs of the cycle are equivalent to ΔG_{expt} and ΔG_{bind} .

Question based on AMS 535:

2. Answer the following questions about amino acid residues from which proteins are made using three letter codes.

- (a) List the 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:

- (b) Indicate which two residues are negatively charged under most conditions.
- (c) Indicate which two residues are positively charged under most conditions.
- (d) Which residue can form disulfide bonds.
- (e) Which residue is incorporated into the protein backbone.
- (f) Which two residues incorporate a "benzene" ring into the side chain.
- (g) Which three residues have "hydroxyl" groups.
- (h) Which charged residue has a planer "guanidinium" group.
- (i) Which residue has a fused two-ring side-chain.
- (j) Which residue has the smallest side-chain.

Questions based on CSE 549:

3. Explain what BLAST or FASTA does, i.e. why might a biologist want to use it.

Then explain algorithmically how it might (ideally does) work computationally.

Questions based on CSE 549:

4. Given two strings v_1 and v_2 , explain how to construct a string w minimizing

$$|d(v_1, w) - d(v_2, w)|$$

such that

$$d(v_1, w) + d(v_2, w) = d(v_1, v_2).$$

$d(.,.)$ is the edit distance between two strings, where each substitution, insertion or deletion costs 1.