

**AMS Common Exam Part B, Computational Biology Track, January 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: Multiple parts**

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

(b) Draw a graph showing the Lennard-Jones Potential. Clearly label all parts of the graph including the axes. Indicate on the graph which parts are attractive and which parts are repulsive. Clearly label the point on the graph which represents the equilibrium distance.

**Question 2: Multiple parts**

(a) Name the 4 major groups of biomolecules.

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(b) Name a commonly used molecular dynamics program.

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(c) Name a commonly used explicit water model.

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(d) Name a commonly used implicit water model.

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(e) Give two examples of data plots (property versus time) often used in molecular dynamics simulation analysis.

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(f) What is a typical time step (with units) used in molecular dynamics simulations.

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(g) There is only one unique set of partial atomic charges that will yield a net formal charge (i.e. +1, +2, -1, -2, etc. (true or false)?

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(h) What does QSAR stand for?

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(i) List the four molecular properties considered in Lipinski's rule of 5.

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(j) How many standard amino-acids are there?

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(k) Name 2 common secondary structure elements.

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(l) Name 2 types of noncovalent interactions that help stabilize folded proteins.

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(m) Name 5 amino-acid side chains (use three letter codes).

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(n) Name 2 hydrophobic side chains (use three letter codes).

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(o) Name 2 hydrophilic side chains (use three letter codes).

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(p) Name 1 negatively charged side chain (use three letter codes).

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(q) Name 1 positively charged side chain (use three letter codes).

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(r) Name the side chain that can form disulfide bonds (use three letter codes).

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(s) Name 2 aromatic side chains (use three letter codes).

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(t) Draw methane.

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(u) Draw ethane.

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(v) Draw methanol.

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(w) Draw benzene.

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(x) Draw water.

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**Question 3:** Explain how genetic sequence data can be used to construct evolutionary relationships between species. Be detailed.

**Question 4:** Describe the BLAST algorithm explaining what it does, how it works, and why it is useful.