

**NAME:**

**Part I: MD Concepts** (20 pts)

1. What are the atomic masses of carbon, nitrogen, oxygen, and hydrogen? (2 pts)
2. What approximation do we make in our simulations in Project 4 regarding atomic mass, and how might this affect the simulation? (3 pts)
3. What are the advantages and disadvantages of coarse-grain vs. fine-grain models? (3 pts)
4. What physical analogy do we use to describe bonds between atoms? (2 pts)
5. Qualitatively, how does the value of  $k_b$  or  $k_n$  affect the way paired atoms behave (describe it in terms of the physical analogy from #4)? (2 pts)
6. In what sense do the non-bonded reference distances act to "summarize" the real forces between atoms? (2 pts)
7. What would happen if we allowed the nonbonded reference distances ( $r_0$ 's) to change as the molecule moved (based on its new configuration) instead of fixing these throughout the simulation? (3 pts)
8. What do we use to measure the overall stability of the structure we are simulating? What are the different contributors to this measurement? (3 pts)

**Part II: Simulations of BPTI** (55 pts)

1. Describe the number and type of secondary structures visible in 6PTI. (Hint: play around with the "Representations" window in VMD.) (3 pts)

2. Briefly describe how the molecule behaves under the following parameter settings (adjectives like 'loose', 'jiggly', 'buzzy', 'calmly undulating', and 'wildly flailing' are valid descriptors). Speed will vary, so slow down the visualization slightly – just a millimeter or two off full speed so you can see the movement more clearly – and describe simulations relative to other ones. Pay attention to side chains and bond lengths, and include details about these if possible. (2 pts each)

**Default:**

**Temp = 50 K:**

**Temp = 1000 K:**

**Temp = 4500 K:**

**$k_b = 100.0$ :**

**$k_b = 10000.0$ :**

**$k_n = 1000.0$ :**

**$k_n = 10000.0$ :**

**Mass = 2.0:**

**Mass = 50.0:**

**$k_b = 100.0$ ,  $k_n = 10000.0$ :**

**nbCutoff = 0.25:**

**nbCutoff = 0.75:**

**(Extra credit)  $k_b = 100.0$ , Temp = 3000 K:**

3. The simulations for the two nbCutoff values (0.25 and 0.75) should look markedly different. Why does changing this parameter result in the observed molecule behaviors? (5 pts)

4. At what size time step does your simulation become completely unstable (i.e. produce overflow errors)? (3 pts)
  
5. What is the general trend in molecule behavior with increasing temperature? (3 pts)
  
6. What is the general trend in molecule behavior with decreasing  $k_b$ ? (3 pts)
  
7. What is the general trend in molecule behavior with increasing  $k_n$ , and why? (3 pts)
  
8. What is the general trend in molecule behavior with increasing atom mass? (3 pts)
  
9. Conceptually, what does reversing the relationship of  $k_b$  and  $k_n$  do? (3 pts)
  
10. In "line" representation (the default in VMD), focus on some of the amino acids with ring systems. What do these rings seem to be doing that goes against what realistic chemistry dictates (this is more evident at more extreme parameter settings)? (3 pts)