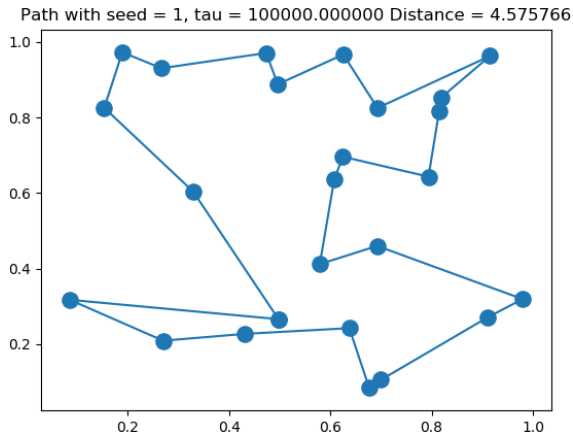
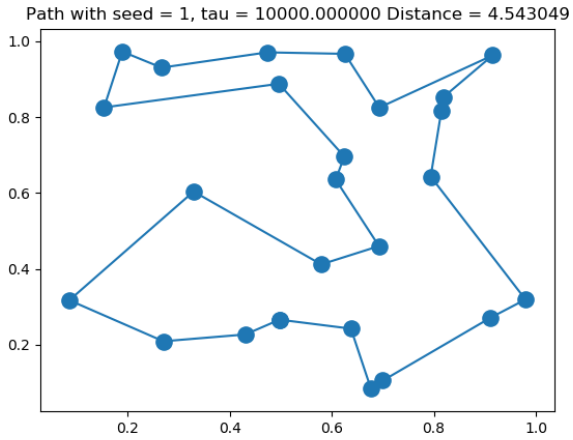
Lab 11 Question 1 and 3 Report

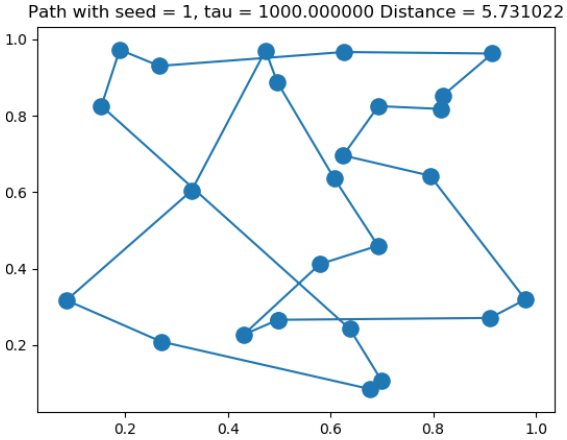
Question 1:

a) Plot with different seeds and tau values, written answer of this question is at the end of the plots.

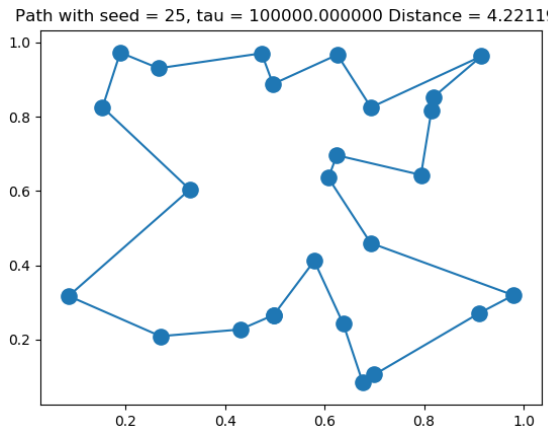
Seed = 1

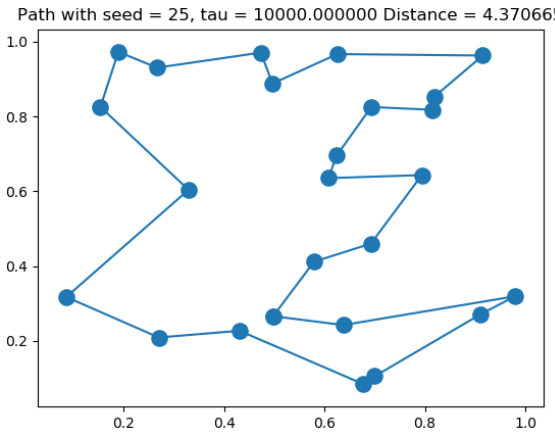


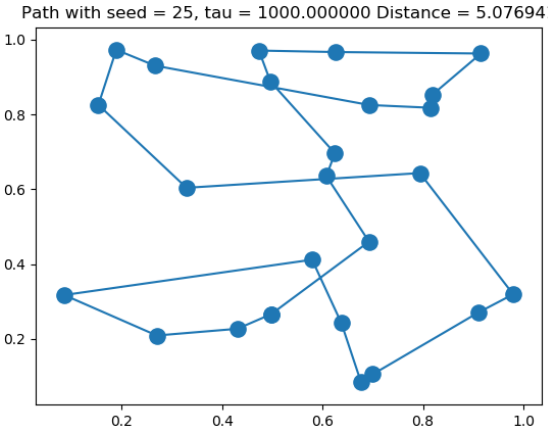




Seed = 25:

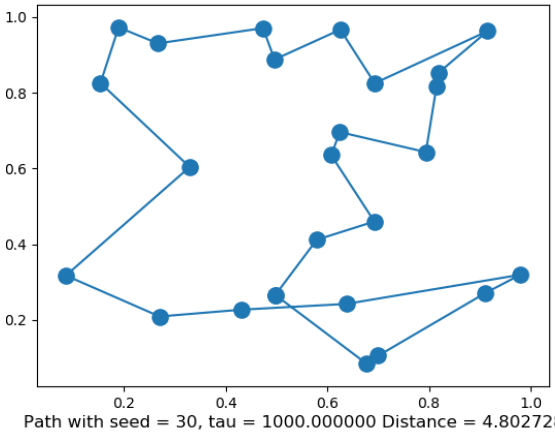

Path with seed = 25, tau = 100000.000000 Distance = 4.221199
1.0
0.8
0.6
0.4
0.2
0.2
0.4
0.6
0.8
1.0


Path with seed = 25, tau = 10000.000000 Distance = 4.370665
1.0
0.8
0.6
0.4
0.2
0.2
0.4
0.6
0.8
1.0

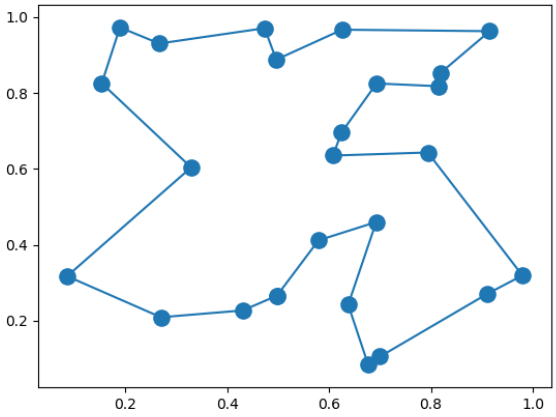

Path with seed = 25, tau = 1000.000000 Distance = 5.076941
1.0
0.8
0.6
0.4
0.2
0.2
0.4
0.6
0.8
1.0

Seed = 30:

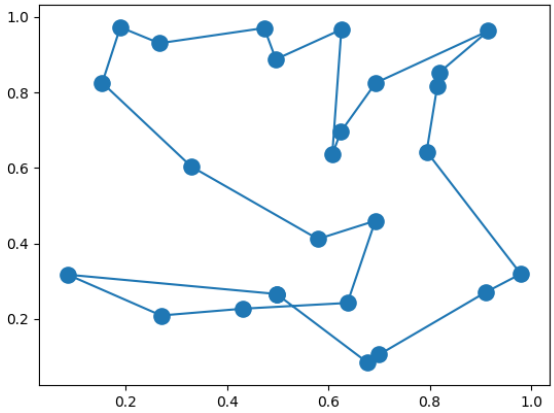
Path with seed = 30, tau = 100000.000000 Distance = 4.418754



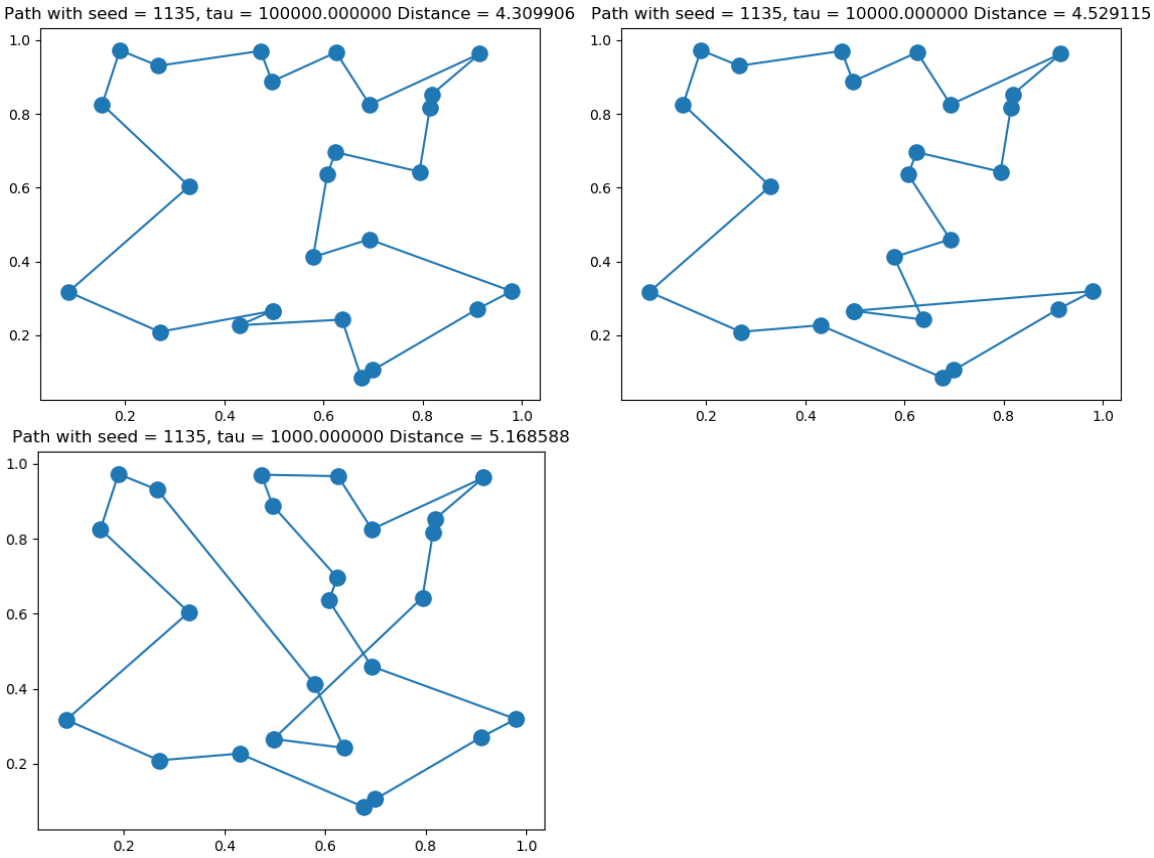
Path with seed = 30, tau = 10000.000000 Distance = 4.221934



Path with seed = 30, tau = 1000.000000 Distance = 4.802728



Seed = 1135:



From the plot, we observed the final path will be smaller if we use a greater tau value. Since tau controls the system's cooling time, a greater tau value will result a slower cooling time for the system. The simulation suggests that longer cooling time will result in shorter path.

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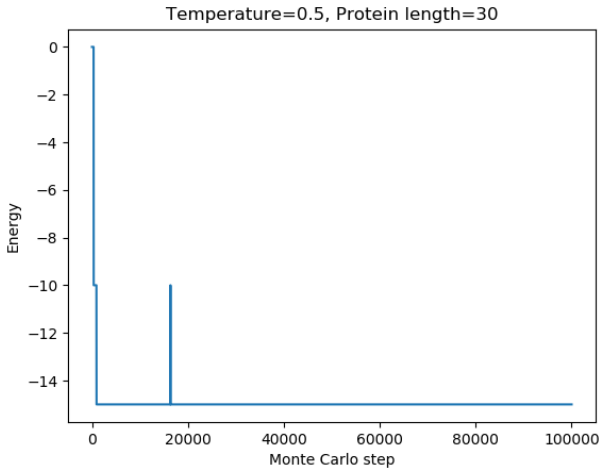
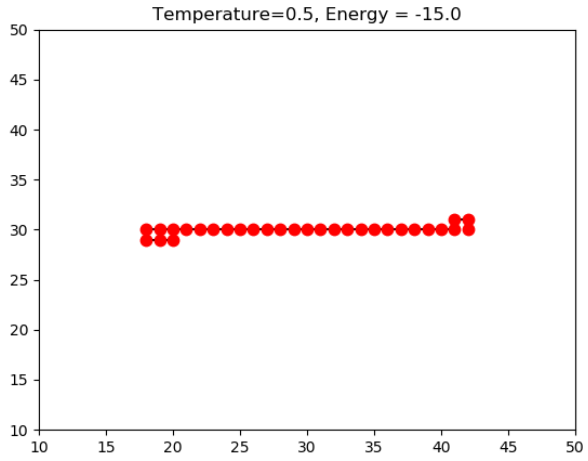
b): Use the program to find the global minimum of equation (19)

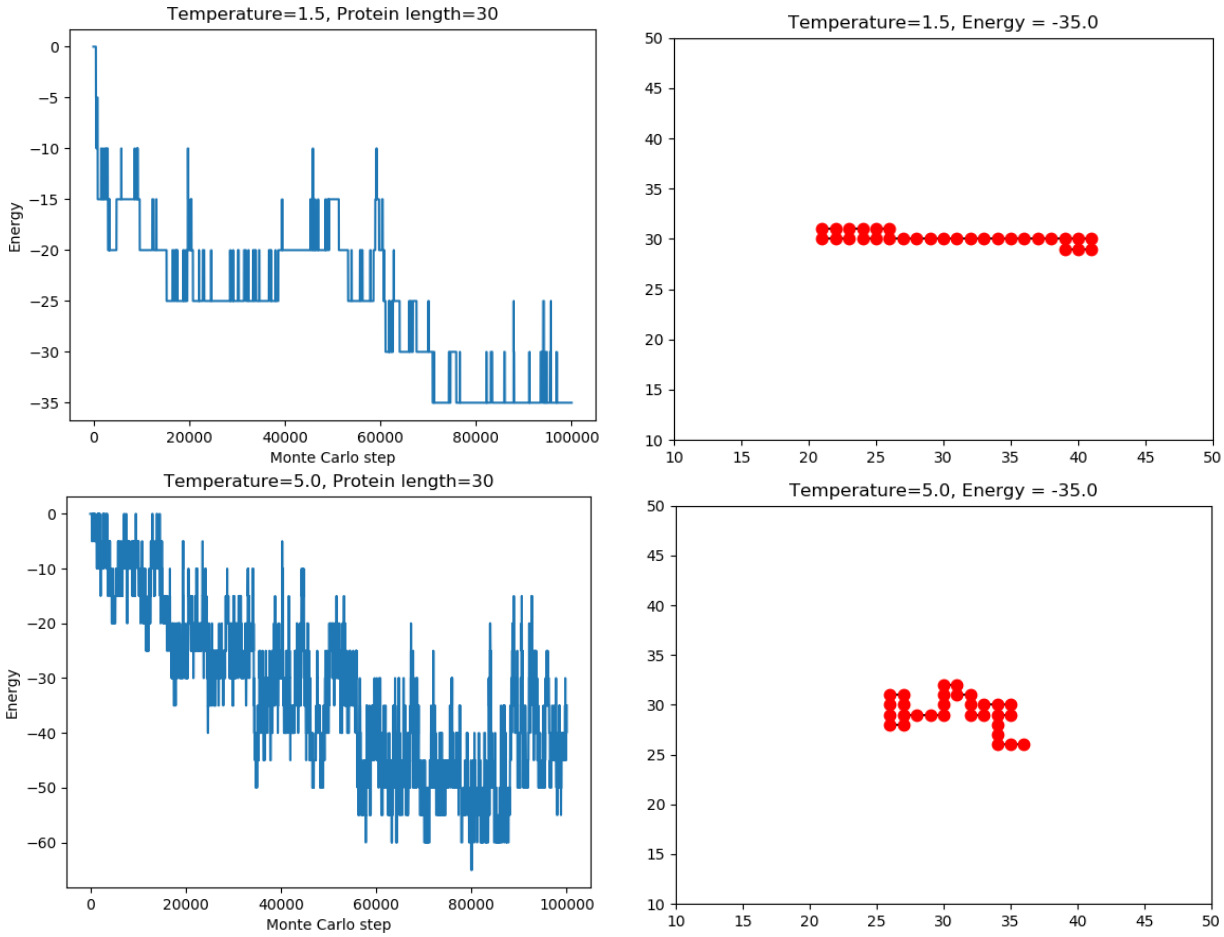
The program in this question is implemented in the file Lab11Q1b.py as method *Question1b()*, the other functions in the file are just helper functions for *Question1b()*. For this simulation, we use (2, 2) as our initial position. The point settles at (2.1581163275978366, 1.0016681594997434) after the simulation ends, which is very close to one of the completing minimums at that region. The converging value of x and y are plotted individually below:

Question 3:

a): Draw the plot with T = 0.5, T = 1.5 and T = 5 and describe the result.

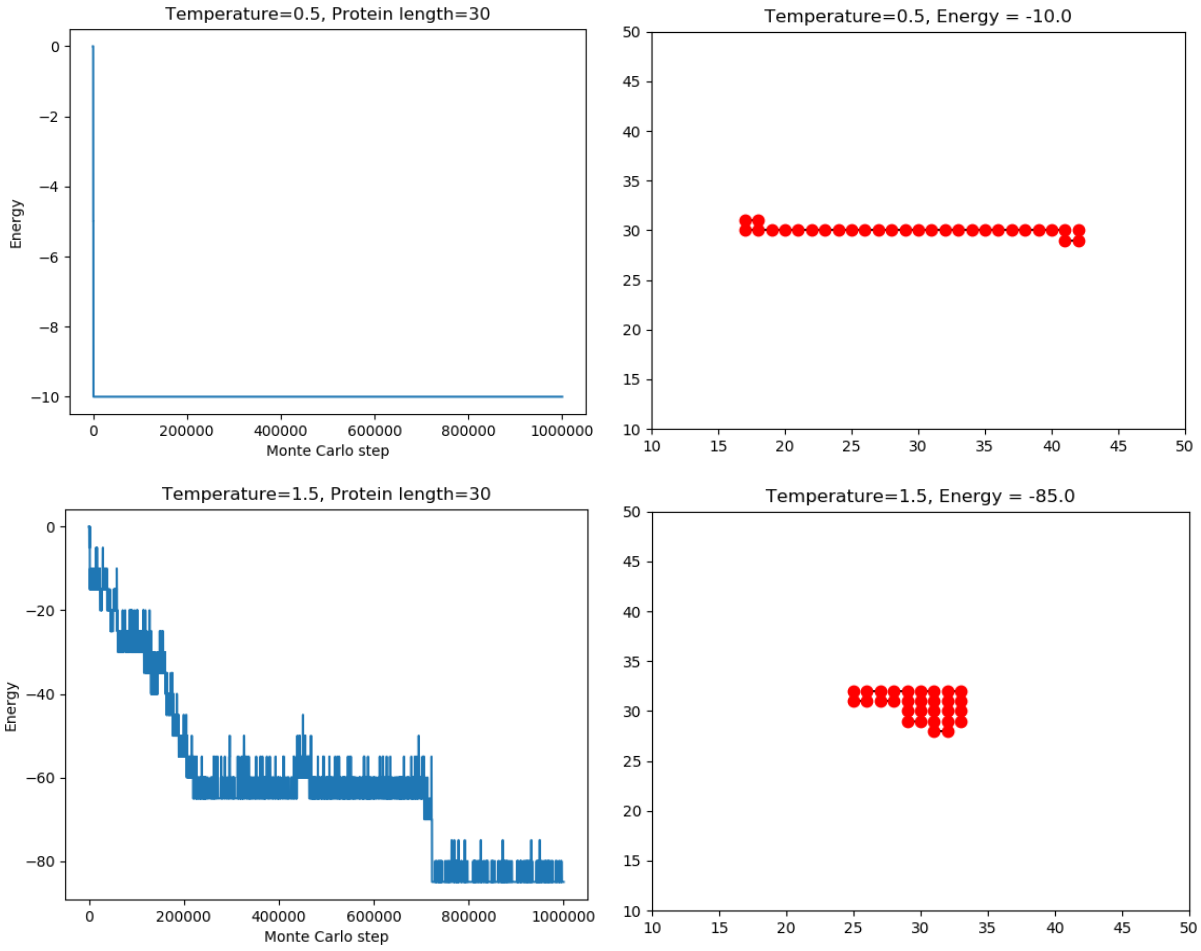






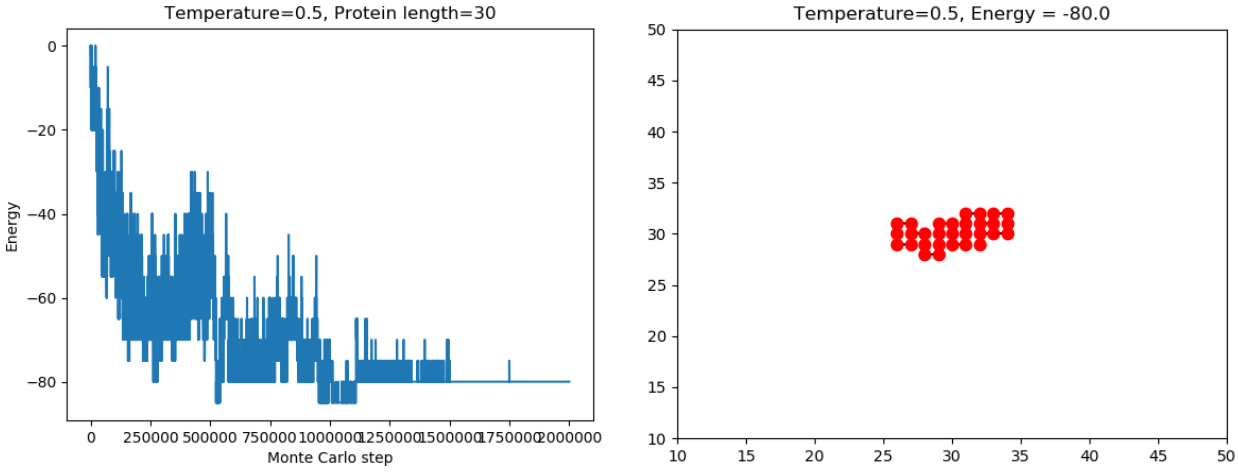
Compare to the folding process at lower temperature, there are more folding happening at higher temperature. Also, when the simulations are over, the energy state of the protein is lower than the simulation with lower temperature. The visual representation of the protein also suggests this conclusion. When simulating with a higher temperature, the protein is more folded together, hence less potential energy.

b):



We expect the energy for case T = 1.5 is lower than the case with case T = 0.5. In T = 0.5 case. Since the temperature is low, the probability of a folding happening is very low. Therefore, the protein at the end of the simulation is largely unfolded, and the energy state of the protein stays high.

c): How does this compare to the T=0.5 simulation from part b where there was no simulated annealing?



The approximate energy for the last quarter of the graph stays at around E = -80 for the simulate annealing. Compare to the graph without simulate annealing, there are more folding happening for the front half of the graph when the temperature is still high.

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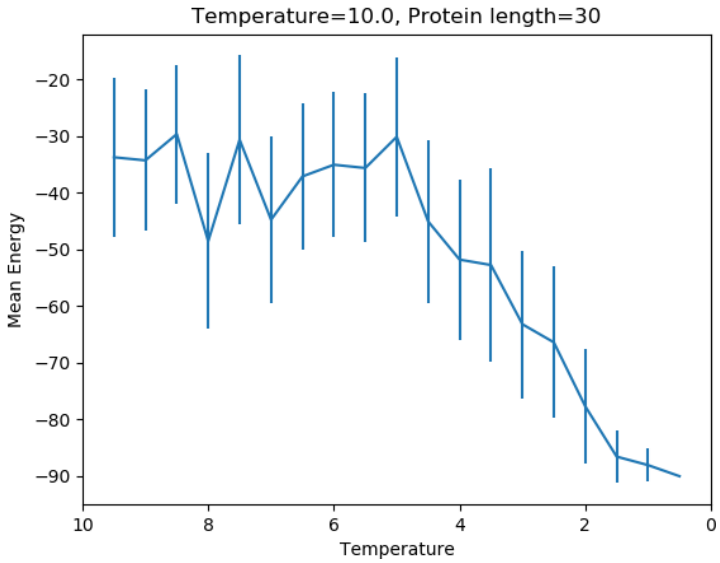
d): Discuss the result from the plot generate from the program.



From the simulation, the final mean energy is around -93, which is around what we expected. In the plot generate by our program, we suspect that there is constant phase transition after Temperature = 5 since there are drastic energy change in a small interval. There are phase transitions also around Temperature = 8. After Temperature = 5, the mean energy states of the system are constantly going to towards the minimum and never bounce back up again, suggesting that the cooling method is working as intended.
