HW5

1.a. FASTA file of the AA sequence(40-650 AA, 200 AA MAX per domain).

b.

c. Job ID: Job 63505; 1 domain; template ID and protein class: [4q57B\_201](http://robetta.bakerlab.org/pdb.jsp?pdbid=4Q57B_201)  ,confidence=0.7812. This is a homology modeling case

2.

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|  | Advantages | Disadvantages | Application Example |
| Centroid | Fast. Less memory consumed. | Not accurate, especially for non-bb atoms interaction prediction. | Low resolution prediction. Predict the backbone rough position and basic secondary structures(S/H/L). |
| Full Atom | More accurate. | Time and memory consuming. | H-bond prediction, and proteins with large side chain groups. Especially important for energy calculation and precise atom placing. |

3. The fragment insertion is much more effective than single torsion angle moves. The small move and shear move can only change a torsion angle one time, and with an ideal angle range. The fragment insertion can give several torsion angles one time, and the angles are more realistic because it considers the different types of amino acids. But the process to generate a 9-mer and 3-mer fragment files is time-consuming and complex.

5. =0.5, delta E=0.9631

6. For the Ab initio modeling, we can compare the lowest score decoy with the native structure to see if they can be matched. Also, the lowest score decoy should have the similar score with the native one. The move map of the algorithm should have the ideal degrees of freedom we want. There should be enough iterations and decoy numbers.

To make an algorithm more effective, we can add the numbers of iterations for both low resolution and high resolution modeling. Also, there should be enough decoys. And consider to use all kinds of movements with reasonable value ranges.

7.

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|  | Iterations | Decoys | Computer time | Total computer time |
| Simons et al. (1999) | 10000 | ~30000 |  |  |
| Bradley et al. (2005) |  |  | 1 min on 1 CPU for a  100-residue protein | 15 processor (3.2 GHz) days. |
| HW4 | 100 | 100 | 10.272017 | 15.760105 |
| HW5 | 3000 low-res  1000 high-res | 10 | 26.047219 |  |

8. Detailed balance: which requires that each transition x→x' is reversible: for every pair of states x, x', the probability of being in state x and transitioning to state x' must be equal to the probability of being in state x' and transitioning to state x, pi(x)P(x\rightarrow x') = \pi(x')P(x'\rightarrow x).

the Metropolis Monte Carlo algorithm generates a new configuration n from a previous configuration m so that the transition probability W(m → n) satisfies the detailed balance condition.

I think the Monte Carlo Object itself satisfies the detailed balance, but the Monte-Carlo-plus-minimization algorithm does not satisfy the detailed balance. There is a larger possibility to accept the movement, since the minimization step will automatically find the lower energy around the movement in the energy landscape. Move m to n, then the acceptance rate P(m to n)> P(n to m).