Probable Questions as per OBE (Open Book Examination)

Q1. Why is modeling solvation important? What is "implicit" versus "explicit" solvation?

Q2. How does the Monte Carlo algorithm work?

Q3. What is the energy gradient? How is the gradient used in energy minimization?

Q4. What is a "local minimum"?

Q5. Why do you always energy minimize before running MD?

Q6. Explain the following:

1. Gradient minimization methods

2. 2nd derivative-based methods

3. Predictor-Corrector Algorithm

4. Born-Oppenheimer Approximation

Q7. How does the conjugate gradient method differ from the steepest descent method?

Q8. Describe the terms of a typical molecular mechanics force field. You should write down the

equation, explain the variables, and explain with words what they represent.

Q9. Describe **all** steps involved in setting up a molecular dynamics simulation of a membrane protein with a ligand. You can assume that there is a crystal structure of the protein with the ligand. The purpose of the simulation is to analyze the dynamics of the protein. Try to be as detailed as possible.

Q10. How is temperature controlled in molecular dynamics and Monte Carlo simulations?

Q11. Describe two techniques used to reduce computational time for molecular dynamics simulations.