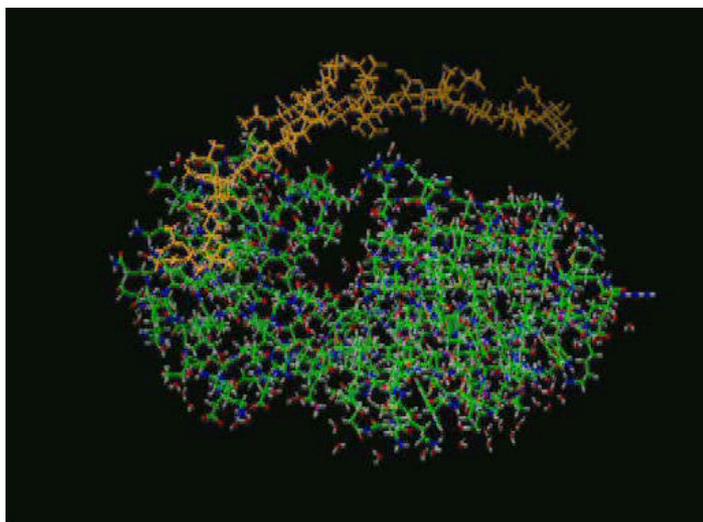


Experimental and Computational Studies of Single-Molecule Enzymatic Reactions: MD Simulation of T4 Lysozyme Conformational Change under Enzymatic Reaction

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- 0.5 ns simulation with 1 fs step size
- Using Discover and CVFF Force Field
- Only crystallographic water included
- Calculated Electrostatic Surface Potential

- 2.0 ns simulations with 2 fs step size
- Solvent water box with counter ions
- With and without ligand using Amber99 force field

Combining single-molecule enzymatic dynamics and molecular dynamics simulation, we have been able to obtain detailed information of the dynamics, mechanism, and energy landscape of T4 lysozyme enzymatic reaction (as a model system). The simulation have clearly showed the hinge-binding motion of the two domains of T4 lysozyme during enzymatic reaction. The rates of each steps of the enzymatic reaction are correlated with the single molecule conformation dynamics.