Molecular Dynamics Simulation of HIV-1 Reverse Transcriptase

Abderrahmane Benghanem[1, 2] and Maria Kurnikova[3]

[1]Bioengineering and Bioinformatics Summer Institute, Department of Computational Biology, University of Pittsburgh, Pittsburgh, PA 15261
[2]Rensselaer Polytechnic Institute, Troy, NY
[3]Carnegie Mellon University, Pittsburgh, PA

HIV-1 reverse transcriptase (RT) has been in the center of attention in the treatment of AIDS for many years. Understanding its structure will prove essentially useful in the design of new antiviral agents. The unliganded structure has been studied by Molecular dynamics techniques showing the flexibility and rigidity of HIV-1 reverse transcriptase. Solving the flexibility of HIV-1 RT is essential in determining controlling mechanisms of polymerases, binding of inhibitors, and developing more efficient drugs in the treatment of AIDS. The AMBER module was used to carry out the molecular dynamics studies. All calculations are performed using AMBER and its force fields as well as the Ptraj analysis package. Harlem, a locally developed simulator, is used for sample preparations and output simulations.