Effects of Salt Concentration on the HIV Rev-RRE Complex using Molecular Dynamics Simulations

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Recognition of the rev responsive element (RRE) by the rev protein is critical to the human immunodeficiency virus (HIV) life cycle, allowing unspliced and partially spliced viral RNA to exit the nucleus. NMR studies have shown increasing salt concentration affects side-chain dynamics. Two NMR structures of the complex were simulated under four different NaCl concentrations with explicit water. Each system (~72,000 atoms) was equilibrated for a minimum of 10.0 ns before statistics were calculated on every 1.0 ps snapshot of a 10.0 ns production run. All systems were converged after 10.0 ns as shown by RMSD plots, and monitoring of structural properties. Hydrogen bonding and arginine side-chain dynamics were examined in all systems. Preliminary analysis suggests agreement with both structural experiments and bioassays. Interestingly, major structural changes do not occur with increasing salt presence. Current analysis focuses on an examination of electrostatics in the presence of increasing salt concentration.