

Molecular Simulations of Viral Leukemia Protein-RNA Interactions

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Human T-cell leukemia virus type-1 (HTLV-1) infects around 10 to 20 million people worldwide, causing a variety of health problems including adult T-cell leukemia. Rex is a viral protein critical for the transition from early to late stages of the viral life cycle. Rex uses an arginine rich-motif to bind to a specific sequence of viral RNA known as the Rex Response Element (RxRE). An in vitro selected RNA aptamer of RexRE has a higher binding affinity to the Rex peptide than the wild-type RNA. Previous studies indicate that R7 and R13 participate in RNA-peptide water networks. The purpose of this study is to better understand the water network interactions with R7K and R13K Rex mutants. Complexes have been simulated under 200 mM KCl with explicit water molecules. The water networks are analyzed in these systems to determine if water binding decreases when R7 and R13 are changed to lysine.