The aim of this diploma thesis was to study interactions between human Rase H enzyme and a natural and modified substrate using molecular dynamics simulations (altogether 9 MD runs ere produced). Conformational preferences of internucleotide linkages (undergoing contacts with the RNase H enzyme) were studied using several versions of the AMBER force field. Either one or two copies of RNase H were included into the simulated system. As the most important DNA-binding residues were recognized Trp93 and Ser101 in the first DNA binding site and Thr49 and Arg47 in the second DNA binding site. Further, the AMBER force field was re-parameterized slightly using ab initio calculations to produce force constants for the modified phosphonate internucleotide linkage. Biologically active version of the modified internucleotide linkage C3-O3-P-C-O5-C5 was able to bind Arg47 using two hydrogen bonds within the 10 ns MD run (even more effciently than in the case of MD runs with natural internucleotide linkages). On the other hand, the biologically inactive C3-O3-C-P-O5-C5 internucleotide linkage lose contacts with Arg47 quickly.