The goal of this diploma thesis was to study interactions of Argonaute (Ago) protein in a complex with nucleic acids. Based on the available crystal structures of full length Argonaute (from A. aeolicus, Aa-Ago) and/or its domains (human PAZ domain, Hs-PAZ), twelve different simulations were computed. Two initial simulations used model of Aa-Ago with either a duplex of DNA/RNA or RNA/RNA. Major difference was in behavior of the PAZ domain (especially its arginine residues), which tolerated the guide DNA in one simulation, but was disturbing the RNA guide strand in the second. Such an interaction could serve as a mechanism of the substrate recognition. In additional simulations (3-9) employing the Hs-PAZ domain, where no disturbance was found in the DNA/RNA hetero-duplex. Different arrangements of the active site geometry as well as empirical parameterizations of Mg2+ ion were probed and analyzed. The DD-catalytic motif plus D683 in Aa-Ago (equivalent to H807 in human Argonaute2) was observed to coordinate the Mg2+ ion in one and two metal ion dependent catalysis models. Highly conserved R570 and E578 created mutual hydrogen bonds and hence stabilized the active site. To make the cleavage irreversible, a role for the first (unpaired) nucleotide from 5'-end of the guide strand was suggested. It lies in a mutual hydrogen bond with mRNA and its destabilization. Homology modeling of human Ago2 (simulations 10-12) was attempted, but failed due to insufficient template similarity, especially in the vicinity of the active site.