In the introductory chapter, the diploma thesis introduces the reader to the most used tools for the human genome editing (ZFN, TALEN, CRISPR). The following chapters describe in detail the methodology of MD simulations and calculations of hydration and binding free energies. In order to perform our calculations in a massively parallel way, an approach was chosen where a large number of short non-equilibrium MD runs are produced in parallel. From these, work values are obtained, from which the value of the equilibrium hydration or binding free energy is then determined using the Crooks-Gaussian Intersection method. The chosen methodology was first tested in the calculations of hydration free energies of nucleic acid bases and amino acid side chains. In the key results chapter, the complex of the transcription factor Zif268 and a short DNA double helix was studied. The effects of point mutations of individual base pairs in the DNA duplex on the binding free energy values were quantified.