

# Investigation of Collective Motions of RNA Helicases Involved in RNA Transport via MD Simulations

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Helicases are motor proteins, which play a crucial role in translation and transcription of RNA/DNA and in the splicing pathway of pre-mRNA to mRNA. Special attention should be given to the detailed mechanistic work of those enzymes, because it is widely unknown. Key parts for understanding the mechanism are the translocation of RNA, the binding and release of ATP/ADP and the resulting conformational changes. Therefore, we will observe the influence of all ligands and co-factors on the different states of the proteins in this work. We will use molecular dynamics simulations on an atomistic level to be able to investigate the collective motions of the helicases Prp2, Prp22, and Prp43. The simulations are carried out with GROMACS and a AMBER force field. The crystal structures were obtained by our collaboration group Ficner et. al. from the University of Göttingen. Still in the early stages of this project, we already collected information about the ATP binding pocket. Important task for the future is to identify the connection between the conformational changes of the main domains, such as ATP pocket, RNA cleft, cofactor binding side etc.