

Abstract:

Classical molecular dynamics simulations were applied on complexes of RNA-dependent RNA-polymerase, Ribonuclease H, Argonaute and Ribonuclease L with chemically modified nucleic acids, which are studied as potential chemotherapeutic agents. Powerful graphics processing units, through which these molecular dynamics simulations were performed, enabled to acquire trajectory length from hundreds of nanoseconds to one microsecond. Molecular dynamics simulations allowed capture differences in binding of various modified nucleic acids to the above mentioned enzymes. These identified differences fitted well with experimental results. It opens the door for rational design of the structure of potential chemotherapeutic agents based on chemically modified nucleic acids.