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Modelling DNA-ligand interactions through variable force field based MD simulations

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In the field of MD simulations, force field refers to as the combination of a set of mathematical formulae and incorporated parameters that are used to evaluate the protein energy as a function of its atomic coordinates over the passage of time. And therefore, the choice of suitable force field to carry out MD simulation is of utmost importance. Apart from literature survey and previously reported results, there is no direct evidence regarding the choice of appropriate force field for a particular system. This entirely depends upon the type of system that is to be simulated and the parameters to be analysed. In the current research article, analysis of molecular dynamics trajectories for ligand-DNA interactions over two such force fields, AMBER03 and CHARMM27 have been done. The functional forms including the parameterization protocols of both the force fields are also studied and well discussed in this research article. It was found that energetics related to CHARMM27 force field are in better agreement with the RMSD of the complex than that of the AMBER03 force field and hence CHARMM27 force field can be a suitable choice to model DNA-ligand complexes for shorter simulations as the convergence criterions are met earlier with minimum or no deviations in the RMS plots.

Keywords: AMBER03, CHARMM27, Force field, Molecular dynamics

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