# Analysis and comparison of force field of RNA using molecular dynamic simulations.

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DNA and RNA are big and flexible polymers that be choice by nature to transmit information. The most common 3D structure is represented by the helix, but these biopolymers are extremely flexible and polymorphic. They can easily change its structure to adapt to different interactions and purposes. RNA has numerous key cellular roles in addition to being the intermediate molecule for the gene expression, as the genetic information stored in DNA is decoded to proteins. In the literature, the proteins remain the most characterized cellular effectors, whilst the pivotal roles performed by RNAs within the cell are more recently being fully appreciated. Despite the great importance of nucleic acid–protein interactions in the cell, our understanding of their physico-chemical basis remains incomplete. Our understanding of the importance of these unusual or transient structures is growing, as recent studies of RNA topology, supercoiling, knotting and linking have shown that the geometric changes can drive, or strongly influence, the interactions between protein and RNA, so altering its own metabolism. In order to address this challenge, we used molecular dynamics simulations (DM) to analyze some standard force fields and new refinement of force field applied in nucleobases of RNA. A comparison against set of available values in the literature and experimental data attests to the quality of the computational approach and the force field. This work is a crucial help in the understanding and planning of natural and artificial nanostructures is given by modern computer simulation techniques, which are able to provide a reliable structural and dynamic description of nucleic acids. The force field will improve usage in various practical applications such as docking, interface design and structure prediction.