Modeling of coarse-grained structures for the RNA nanotube using molecular dynamics simulation

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The self assembly of the RNA nanostructures is straightforward due to high flexibility of RNA molecules. We construct the novel RNA nanoclusters- the RNA nanotubes made of several nanorings. We study the structural properties (i.e., the Root Mean Square Deviation (RMSD), the radius of gyration and radial distribution function (RDF)) of such RNA nanotubes up to the size of about 20nm in physilogical solutions that can be used for drug delivery into the human body. We model RNA nanotubes by utilizing the molecular dynamics simulation method implemented in NAMD and VMD. Furthermore, we calculate the histograms for the bond angles and the dihedral angles. From dihedral angle histogram we see the characteristics of the links used to build the nanotube. Using these all-atom MD simulation results we develop the coarse-grained models which lead to a possibility of explaining the properties of complex biological systems at large scales. For the coarse-grained structures we have performed the Molecular dynamics simulation using DL-POLY to calculate the radial distribution function. We also present the root mean square deviation for the system of the coarse-grained model to demonstrate the equilibration of the system. The change in these features with the size of the nanotube will be discussed.