Coupled Rings in RNA Nanotubes and Properties of Biological Nanoclusters

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ABSTRACT

In this contribution, we study biological nanoclusters where the coupling between their parts is essential. The main focus is on RNA-based nanostructures. RNA molecules are very flexible in nature. This feature allows us to build various motifs which are essential in bio-nanotechnological applications. Based on the previous studies on RNA nanorings [1, 2], in this contribution we analyze the structure and properties of RNA nanotubes, where we focus on nanotubes consisting of a series of coupled nanorings of around 20nm in diameter. We have developed a molecular dynamics (MD) method and implemented it by using the NAMD and VMD packages to study the structural and thermal properties of the nanotube in physiological solutions. In order to achieve realistic temporal scales, we have subsequently developed a new coarse-grained methodology for this type of biological nanostructures. We provide all details for our three-bead coarse-grained model for which we calculate the histograms for the bond angles, as well as for the dihedral angles. From the dihedral angle histogram we can analyze the characteristics of the links used to build the nanotube, and therefore coupling effects.

We have analyzed such characteristics as the Root Mean Square Deviation (RMSD), the radius of gyration, the number of hydrogen bonds per base pairs, and the radial distribution function for the different nanoclusters in nanotubes of various sizes. The variations of energy and temperature with simulation time have been studied for all sets of simulations. We have calculated the bead distances along the chains of RNA stands in nanoclusters. The change in these features with the size of the nanotube is a key to understanding the coupled effects in these structures. Finally, we have confirmed the process of ion evaporation with temperature decrease. This is due to the phenomenon of self-stabilization, first reported in [2].

REFERENCES

[1] Y. G. Yingling, B. A. Shapiro, Computational design of an RNA hexagonal nanoring and and RNA nanotube, *NanoLett.*, 7, 2328–2334 (2007).

[2] M. Paliy, R. Melnik, B. A. Shapiro, Molecular dynamics study of the RNA ring nanostructure: a phenomenon of self-stabilization, *Phys.Biol.*, 6, 046003 (2009).