Supporting Information

Atomic Structures of RNA Nanotubes and comparison with DNA nanotubes

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Section 1: Design of The RNTs

Figure S1. The structure of the RNT is built using NAB of AmberTools16. (a) RNT1: The design of crossovers and nicks are same as DNT as previously reported\(^1\). Only the thymine is replaced by uracil. (b) RNT2: The structure is taken from experimental design by Endo et. al.\(^2\). The structure is a portion of the original RNA origami Nanotube. RNT1 has 57bp dsRNA per helical domain whereas RNT2 has 56bp dsRNA per helical domain. Different color represents different staple strands.
Section 2: Cross-sectional Area of Moment of Inertia (AMI) of the RNTs

The second moment of inertia or Cross-sectional area of moment of inertia for an arbitrary shape V with respect to a given axis ZZ’ is defined as,

\[ I_{ZZ'} = \iint_A r^2 dA \]

Where, \( r \) is distance of the infinite small area element \( dA \).

Assuming, dsRNA as a cylindrical tube we can write the AMI of a single dsRNA with respect to the long axis as following,

\[ I_{ZZ'} = I_0 = \frac{\pi R_1^4}{4} \]

Now, according to the parallel axis theorem, the AMI for RNT consisting of 6 dsRNA arranged in hexagonal manner with respect to the long axis is \( 1.5 \).
In our all analysis, we took $R_1 = 1.125 \text{ nm}$. To calculate $R_2$, we average the pore radius of the RNTs.
Section 3: Definition of Slice and Segments

Figure S2. (a) Definition of Slice used for different analysis. Each RNT is composed of six 57-mer (RNT1) or 56-mer (RNT2) ds-RNA. So, the RNT is divided into 57/56 slices containing 1 bp from each helical domain. (b) To define segments, we divide the RNTs into 9 parts. Each part contains 7 bp per helical domain except the terminal ones, which have 4 bp per helical domain. For RNT2 the middle segment has 1 less bp per helical domain. Different color represents different segments.
Section 4: Comparison of radius profile of DNT and RNTs

Figure S4. Radius of the pore of RNT1, RNT2 and DNT.
### Section 5: RNTs in charge neutral Mg\(^{2+}\) and 10mM of MgCl\(_2\) Solution

#### Details of the Systems

<table>
<thead>
<tr>
<th>Type of the RNT</th>
<th>Box dimension [Å]</th>
<th>Total No. of Atoms</th>
<th>No. of Mg(^{2+}) added to neutralize</th>
<th>No. of Cl(^-)</th>
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<tbody>
<tr>
<td>RNT1 in charge neutral Mg(^{2+})</td>
<td>[118.9×125.5×234.6]</td>
<td>299857</td>
<td>333</td>
<td>-</td>
</tr>
<tr>
<td>RNT2 in charge neutral Mg(^{2+})</td>
<td>[118.9×125.5×232.1]</td>
<td>296720</td>
<td>328</td>
<td>-</td>
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<tr>
<td>RNT1 in 10mM of MgCl(_2) Solution</td>
<td>[118.9×125.5×234.6]</td>
<td>299731</td>
<td>354</td>
<td>42</td>
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<tr>
<td>RNT2 in 10mM of MgCl(_2) Solution</td>
<td>[118.9×125.5×232.1]</td>
<td>296594</td>
<td>349</td>
<td>42</td>
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</tbody>
</table>
RMSD and RMSF

**Figure S4.** RMSD of the different RNTs in charge neutral Mg\(^{2+}\) solution and 10mM MgCl\(_2\) solution. RMSD is calculated with respect to the energy minimized structure.

**Figure S5.** RMSF of the RNTs as a function of Slice Index.
**Radius of the Pore**

*Figure S6.* Radius of the pore of RNT1 in charge neutral Mg\(^{2+}\) solution.

*Figure S7.* Radius of the pore of RNT1 in 10mM MgCl\(_2\) solution.
Figure S8. Radius of the pore of RNT2 in charge neutral Mg$^{2+}$ solution.

Figure S9. Radius of the pore of RNT2 in 10mM MgCl$_2$ solution.
Reference

