Supporting Information

Atomic Structures of RNA Nanotubes and comparison with DNA nanotubes

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Section 1: Design of The RNTs

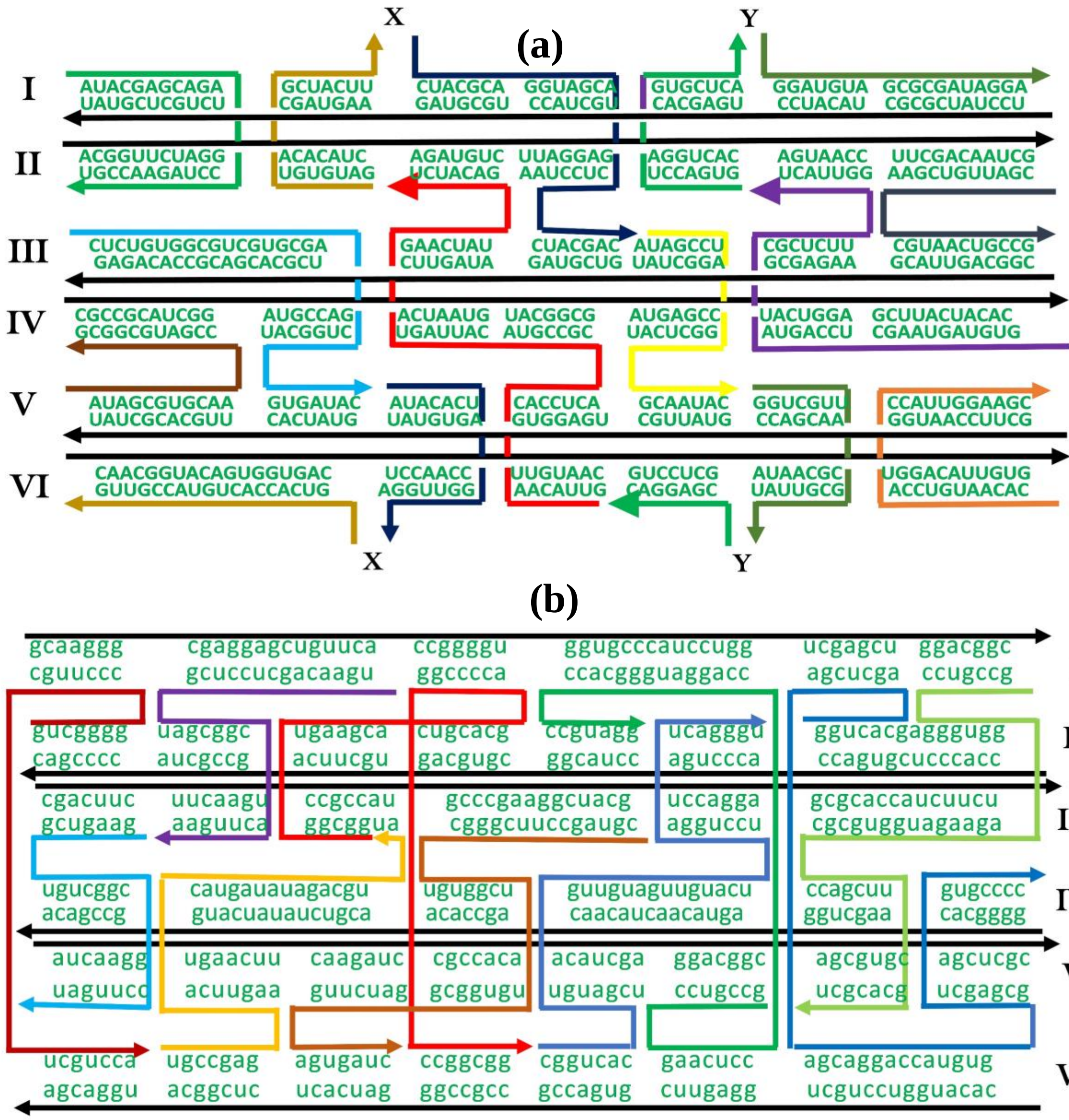
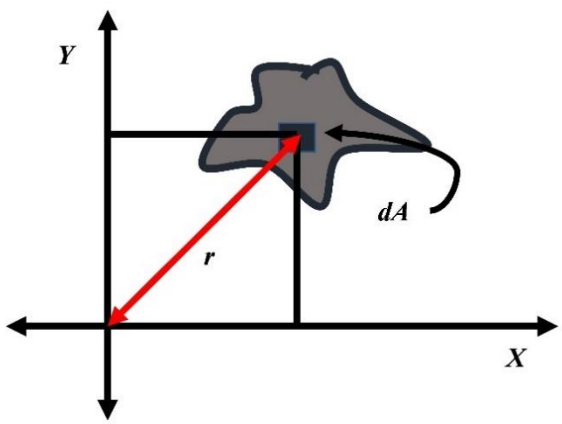


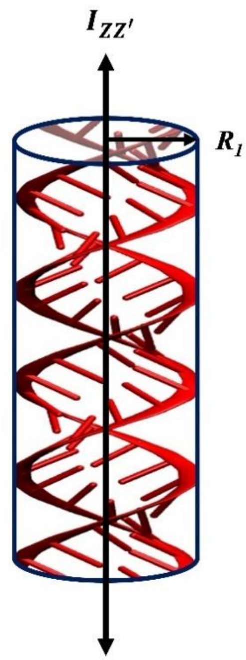
***Figure* S1.** The structure of the RNT is built using NAB of AmberTools16. (a) RNT1: The design of crossovers and nicks are same as DNT as previously reported[1]. Only the thymine is replaced by uracil. (b) RNT2: The structure is taken from experimental design by Endo et. al.[2]. The structure is 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,

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





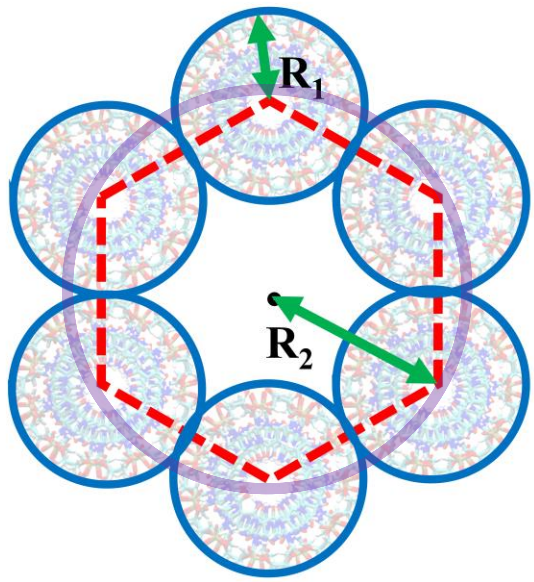
Where, r is distance of the infinite small area element dA.

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

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

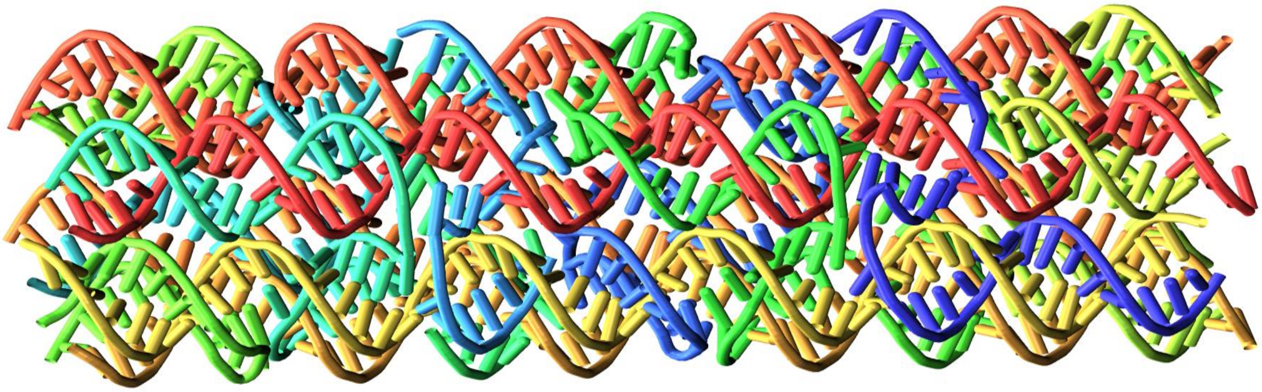
Now, according to the parallel axis theorem, the AMI for RNT consisting of 6 dsRNA arranged in hexagonal manner with respect to the long axis is[1, 3],

$$I = \frac{1}{2}\left[\sum_{6} I_0 + (4R_1^2 + 2R_2^2)A_1 + I_0(16\frac{R_2^2}{R_1^2} - 10)\right]$$



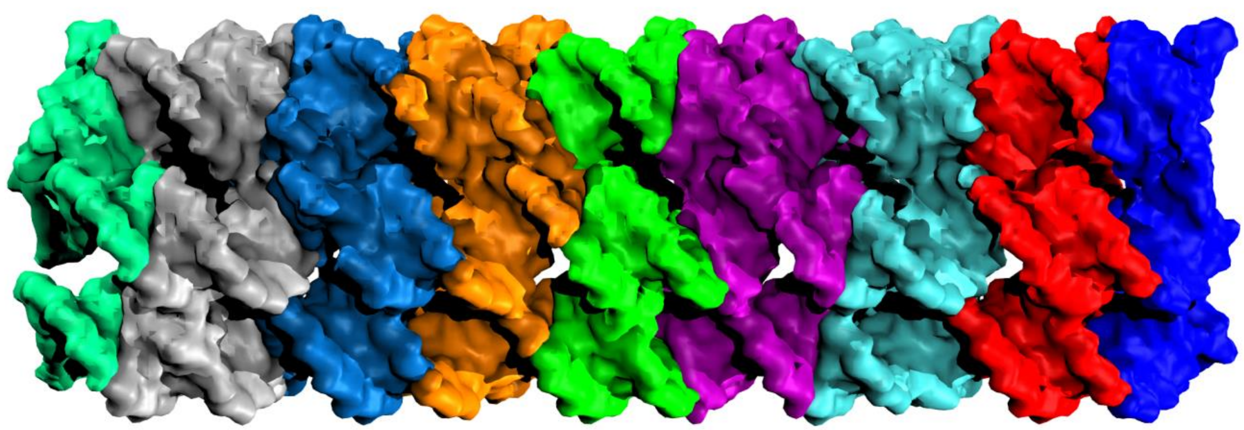
In our all analysis, we took $R_1 = 1.125\ nm$. To calculate R_2, we average the pore radius of the RNTs.

Section 3: Definition of Slice and Segments



1 2 3 4 5 6 ………………………………………………………………………………56 57 58 59

(a) Slice Index



1 2 3 4 5 6 7 8 9

(b) 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

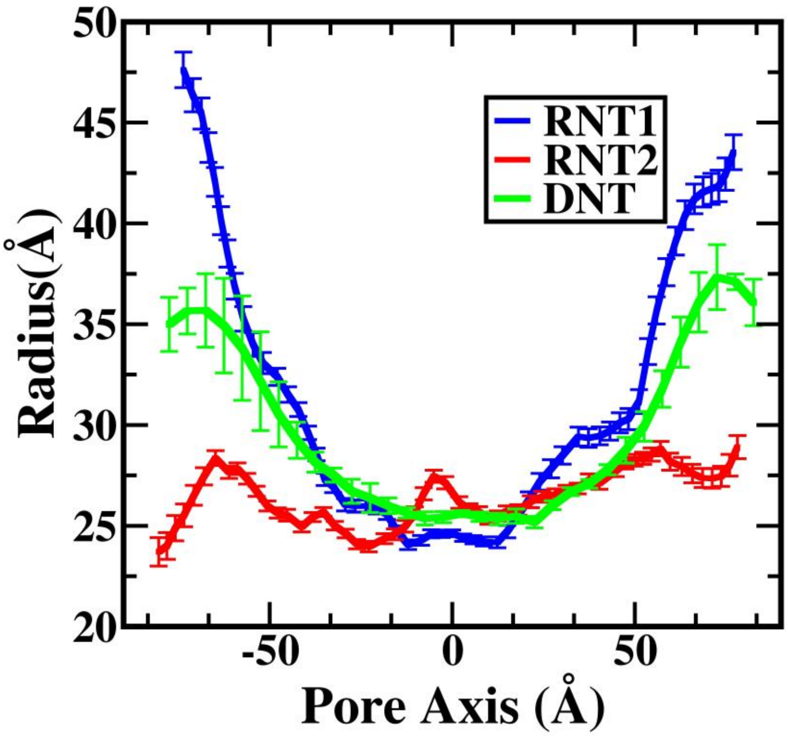


Figure S4. Radius of the pore of RNT1, RNT2 and DNT.

Section 5: RNTs in charge neutral Mg^{2+} and 10mM of $MgCl_2$ Solution

Details of the Systems

Type of the RNT	**Box dimension [Å]**	**Total No. of Atoms**	**No. of Mg^{2+} added to neutralize**	**No. of Cl^-**
RNT1 in charge neutral Mg^{2+}	[118.9×125.5×234.6]	299857	333	-
RNT2 in charge neutral Mg^{2+}	[118.9×125.5×232.1]	296720	328	-
RNT1 in 10mM of $MgCl_2$ Solution	[118.9×125.5×234.6]	299731	354	42
RNT2 in 10mM of $MgCl_2$ Solution	[118.9×125.5×232.1]	296594	349	42

RMSD and RMSF

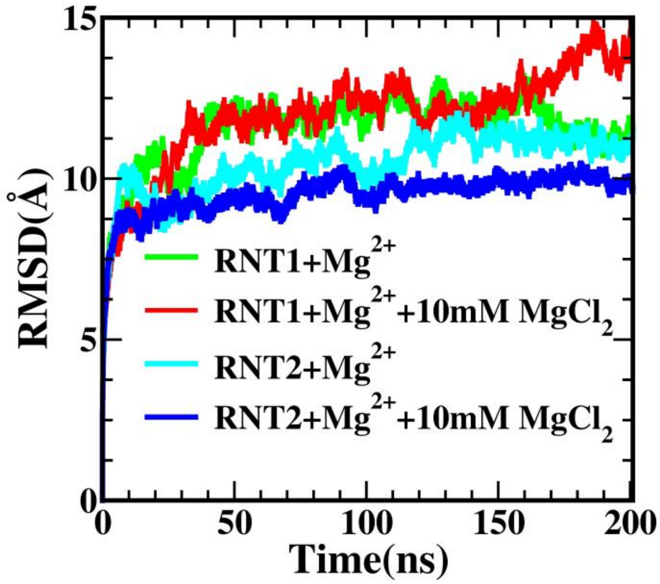


Figure S4. RMSD of the different RNTs in charge neutral Mg^{2+} solution and 10mM $MgCl_2$ solution. RMSD is calculated with respect to the energy minimized structure.

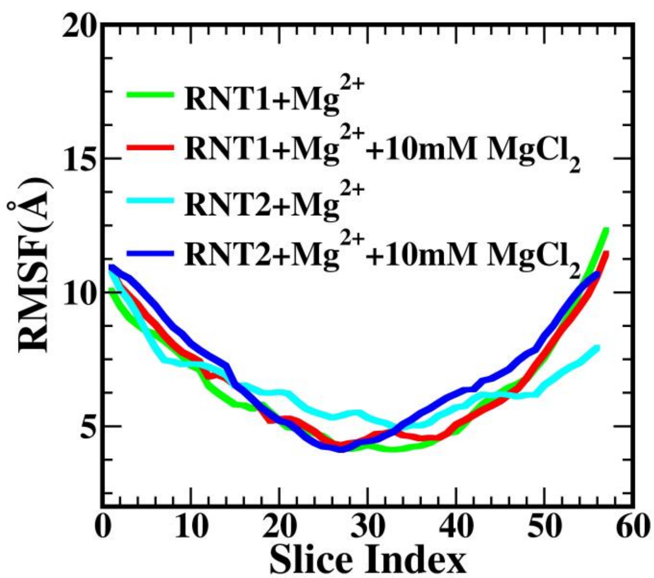


Figure S5. RMSF of the RNTs as a function of Slice Index.

Radius of the Pore

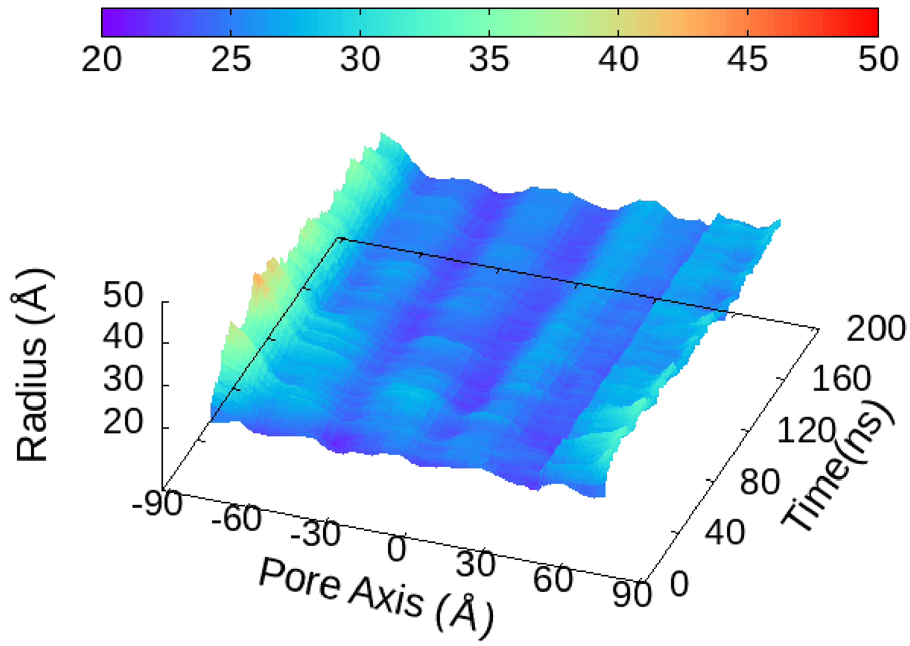


Figure S6. Radius of the pore of RNT1 in charge neutral Mg^{2+} solution.

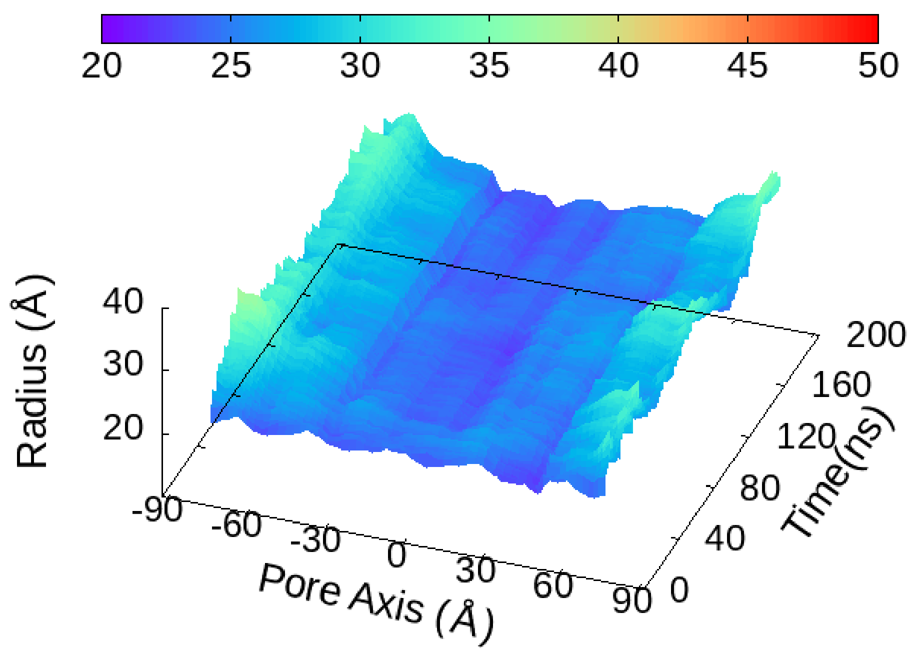


Figure S7. Radius of the pore of RNT1 in 10mM $MgCl_2$ solution.

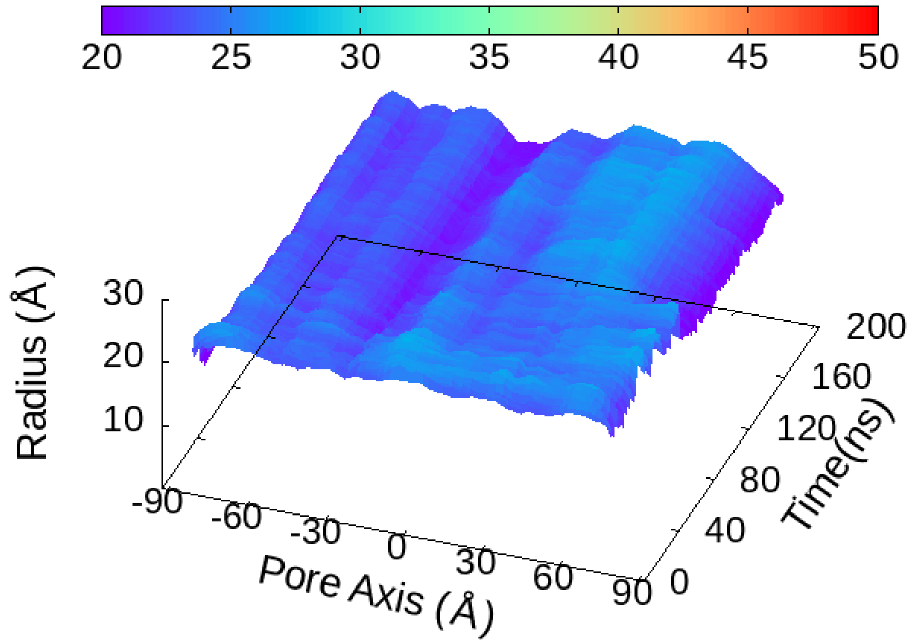


Figure S8. Radius of the pore of RNT2 in charge neutral Mg^{2+} solution.

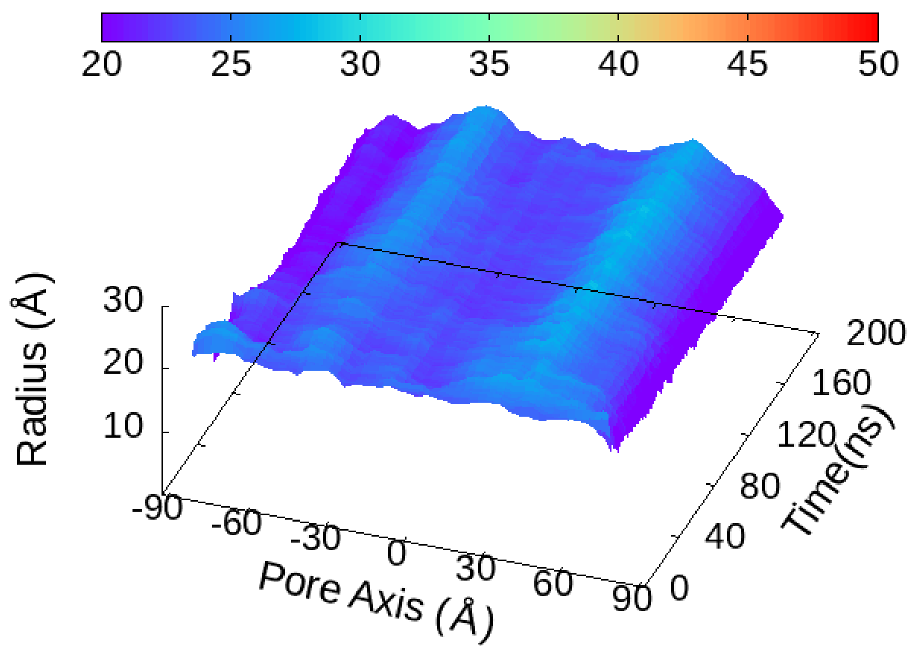


Figure S9. Radius of the pore of RNT2 in 10mM $MgCl_2$ solution.

Reference

1. T. Wang, D. Schiffels, S. Martinez Cuesta, D. Kuchnir Fygenson and N. C. Seeman, *Journal of the American Chemical Society*, 2012, **134**, 1606-1616.
2. M. Endo, Y. Takeuchi, T. Emura, K. Hidaka and H. Sugiyama, *Chemistry–A European Journal*, 2014, **20**, 15330-15333.
3. H. Joshi, A. Kaushik, N. C. Seeman and P. K. Maiti, *ACS nano*, 2016, **10**, 7780-7791.