

CS 590 Homework 1: Designing a novel DNA Nanostructure

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February 2016

1 Introduction

CADNano software was used to obtain a sequence for a proposed nanobot with semi-articulated limbs, consisting of a 4-helix body with two limbs. Two limb variants were created: one with a single helix, the other consisting of two helices. Of this second limb, two designs of differing length were explored.

2 Procedure

Sequence information was exported to CanDo to obtain 3-dimensional structure with atomic level resolution. UCSF Chimera software was then used to view a heatmap of molecular flexibility.

We investigated structural modifications to see their effects on flexibility, first by seeing the effect of doubling the width of the robotic arm, then by seeing the effect of increasing length of the arm.

3 Data

3.1 Effect of increasing length of robot arm

The heatmap revealed areas of greater flexibility closer to the free ends of the limbs.

Interestingly, the heatmap produced by CanDo indicated greater flexibility in Limb 1 (single helix) when Limb 2 was longer. It is difficult to interpret this result further without access to the modeling algorithm used by CanDo. We hypothesized that Limb 1 should have greater flexibility when nearby Limb 2 is shorter as a result of decreased steric hindrance (possibly, CanDo does not take this into account with their model).

Further investigations might involve attachment of small molecules using the CanDo MATLAB scripts to obtain quantitative values for accessible volume. Moreover, the binding propensity of various small molecule and DNA linkers

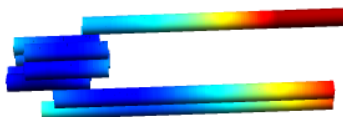


Figure 1: 1- vs 2-helix arms

between the limbs could be investigated using a molecular dynamics package such as VMD/NAMD/Espresso.

3.2 Effect of doubling width of robot arm

The heatmap revealed greater flexibility in the 2-helix limb as compared to the single-helix limb.

References

- [1] DN Kim, F Kilchherr, H Dietz, M Bathe. Quantitative prediction of 3D solution shape and flexibility of nucleic acid nanostructures. *Nucleic Acids Research*, 40(7):2862-2868 (2012).
- [2] CE Castro, F Kilchherr, DN Kim, EL Shiao, T Wauer, P Wortmann, M Bathe, H Dietz. A primer to scaffolded DNA origami. *Nature Methods*, 8: 221-229 (2011).

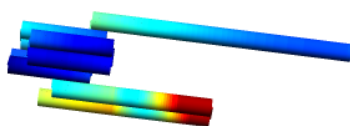


Figure 2: 1- vs 2-helix arms

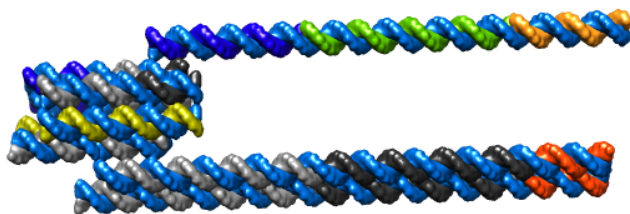


Figure 3: 1- vs 2-helix arms

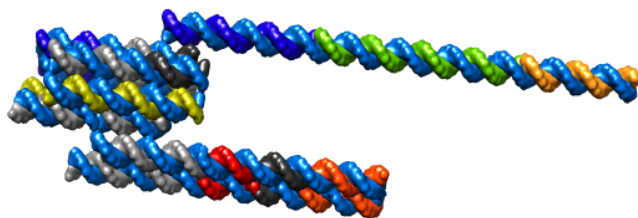


Figure 4: 1- vs 2-helix arms

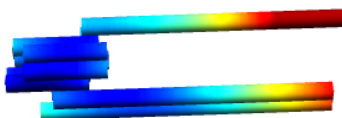


Figure 5: 1- vs 2-helix arms

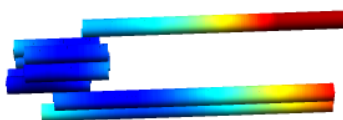


Figure 6: 1- vs 2-helix arms

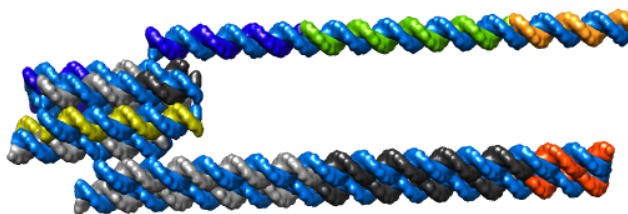


Figure 7: 1- vs 2-helix arms in atomic resolution