1-1-2013

Exploration of the Structural and Energetic Landscape of Glycol Nucleic Acids

Emily A. Sleeman
Concordia University - Portland

Follow this and additional works at: http://commons.cu-portland.edu/suri_msd

Part of the Chemistry Commons

Recommended Citation
http://commons.cu-portland.edu/suri_msd/5

This Poster is brought to you for free and open access by the Summer Undergraduate Research Institute (SURI) at CU Commons. It has been accepted for inclusion in Math & Science Department (SURI) by an authorized administrator of CU Commons. For more information, please contact libraryadmin@cu-portland.edu.
1. Introduction

Glycol nucleic acid (GNA) is a non-natural analog of DNA. In place of the deoxyribose unit of DNA, GNA has an acyclic ethylene glycol unit (Fig. 1). The differences between DNA and GNA are evident in the duplex structure (Fig. 3). Instead of a major and minor groove, GNA has one large groove (Fig. 3). The base pairs of GNA wrap around the single groove like a ribbon on a spool (Fig. 3). GNA has primarily intra-strand base stacking, with each base stacking on top of a base of the opposite strand, as opposed to the inter-strand base stacking of DNA (Fig. 2).

2. Objectives

- Measure forces of extension and separation of GNA relative to identical sequences of DNA.
- Explore structure, flexibility, and energetics of GNA and how these may relate to its stability.
- Explore the usefulness of Steered Molecular Dynamics simulations in investigations of GNA.

3. Methods

Models were prepared for simulation by addition of sodium ions to balance the negative charges of the phosphate backbones, as these charges can make simulations unstable (Fig. 3). Charge-balanced models were then submerged in a water box slightly longer than twice the length of the molecule as determined from crystal structures (Fig. 3).

4. Results

Stretching simulations went mostly as planned. Molecules began to unwind as forces were applied. Hydrogen bonds broke, beginning near the end being pulled (Fig. 5).

- For 16 base-pair duplexes, the same relationship seems to occur as in the 8 base-pair duplexes (Fig. 8).
- Initial simulations were on too short of a time scale to fully separate strands, but it is expected that both curves will peak and fall similarly to the 8 base-pair duplexes once further data is collected.

5. Discussion

- Force measurements appear to differ significantly between GNA and DNA, though further research is needed to clarify details.
- Molecular dynamics appears to be a promising method of study GNA.
- Since GNA appears to move randomly in a spring-like motion, the GNA models in this simulation may not have been in their most compact conformations; more research is needed to see what effect this may have.

6. Current & Future Research

- Further pulling at much slower speeds for more accurate measurements.
- Adaptive biasing force simulations to collect data for free energy calculations.
- Extracting helicaloid parameters of GNA.

7. References


8. Acknowledgements

The author wishes to thank Dr. Andrew Johnson for his support and guidance and the Summer Undergraduate Research Institute (SURI) for funding the project.