Calculating the Melting Temperature of Linker DNA

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Abstract

We created a program which addresses the intrinsic relationship between a DNA sequence and its subsequent melting temperature. The purpose of our program was to find the melting temperature of any given DNA sequence and return a DNA sequence which matches a desired melting temperature.

Our algorithm assists users by providing a consistently error-free sequence generator to form the building blocks of DNA origami. With our algorithm, chemists and students alike can quickly and efficiently find the correct DNA sequence to match a desired melting temperature. Because the Chemistry department at Simpson College has invested heavily in DNA origami research, our program will be instrumental to their studies and eventual findings.

What is DNA Origami?

DNA origami is the process of folding DNA strands into two or three dimensional shapes. This process is performed at the nanoscale level and requires precision in order to create a desired shape. Ultimately, these origami structures can be developed into nanoscale capsules which could theoretically deliver various types of medicine, including chemotherapy. In DNA origami, the assembly of multiple 2D DNA structures into a 3D structure is facilitated by a Linker DNA. Consequently, the binding strength of the DNA origami structures depends on the melting temperature of the Linker DNA sequences. We explored the correlation between a pre-defined DNA sequence and its melting temperature for the purpose of eventually stabilizing the origami structures.

Algorithm

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Every DNA strand is composed of AT and CG pairs. Our algorithm modifies a given DNA sequence by manipulating the character sequence of the DNA strand. Specifically, the melting temperature of a DNA strand is dependent on the number of CG pairs within that sequence. Our algorithm replaces AT pairs with CG pairs (or CG pairs with AT pairs) to meet a desired melting temperature.

Testing and Testing Results

We created randomly computer-generated DNA sequences of various lengths to test our algorithm. The results of our testing are shown in the figure below.



Figure 1: The figure shows the relationship between the length of an individual sequence and increment adjustments. For example, a sequence of 30 bases will experience a change of 1.3 degrees for every base change.

We found that the increments at which we can change the melting temperature of a DNA sequence are wholly dependent on the length of the sequence. If the given sequences are relatively small, our algorithm could not always return a sequence of that length with the desired melting temperature. Inversely, our algorithm frequently found a DNA sequence with the desired melting temperature for larger given sequences. When a sequence with the exact melting temperature could not be found, our algorithm returned a DNA sequence with the closest possible melting temperature.

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