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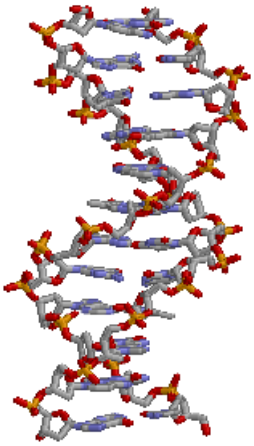
Onoe Hiroaki & Takahashi Hidetoshi's course - 2020

Biomimetic Micro/Nano Engineering
Report 5



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Contents

1 Introduction

DNA is a double helix macromolecule coding for the genetic information of living organisms. It is contained in the nucleus of the cells. Its structures, replication mechanism, how it binds and the fact that it conveys information make it a really interesting molecule for designing nanosystems. Using DNA, researchers were already able to create logic gates, nanostructures, sensors or even actuators. The first part of this report will be dedicated to the thermodynamic behavior of simple, small strands of DNA. Those informations are useful for understanding why DNA strands hybridize or just denature. The second part is my self opinion about the future of DNA nanotechnologies and the possible output to the industry.

2 Assignment 1

2.1 Calculation of ΔG for the following two DNA sat both 300K (26.9°) and 350 K (76.9°C)

Figure 1 represent the two strands for which the thermodynamics properties are investigated.

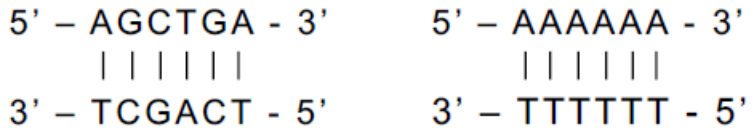

Figure 1: Small strands of DNA [2]

2.1.1 First strand of DNA, left strand on figure 1

The computation of ΔH^* in $[kcal * mol^{-1}]$ is executed as follow :

$$\Delta H^* = \Delta H_{AG/TC} + \Delta H_{GC/CG} + \Delta H_{CT/GA} + \Delta H_{TG/AC} + \Delta H_{GA/CT} + 2\Delta H_{AT-term} \tag{1}$$

Using the Santalucia's parameters, the following value is obtained :

$$\Delta H^* = -37.5 \ [kcal * mol^{-1}] \tag{2}$$

Then the computation of ΔS^* in $[cal * mol^{-1} * K^{-1}]$ is executed as follow :

$$\Delta S^* = \Delta S_{AG/TC} + \Delta S_{GC/CG} + \Delta S_{CT/GA} + \Delta S_{TG/AC} + \Delta S_{GA/CT} + 2\Delta S_{AT-term} \tag{3}$$

Using the Santalucia's parameters, the following value is obtained :

$$\Delta S^* = -103.1 \ [cal * mol^{-1} * K^{-1}] \tag{4}$$

$$\Delta S^* = -0.1031 \ [kcal * mol^{-1} * K^{-1}] \tag{5}$$

The computation of ΔG^* in $[kcal * mol^{-1}]$ is executed as follow :

$$\Delta G^* = \Delta H^* - T\Delta S^* \tag{6}$$

With T = 300K and the values found above $\Delta H^* = -37.5\ [kcal * mol^{-1}]$ and $\Delta S^* = -0.1031\ [kcal * mol^{-1} * K^{-1}]$:

$$\Delta G^*_{300} = -6.57\ [kcal * mol^{-1}] \tag{7}$$

With T = 350K and the values found above $\Delta H^* = -37.5\ [kcal * mol^{-1}]$ and $\Delta S^* = -0.1031\ [kcal * mol^{-1} * K^{-1}]$:

$$\Delta G^*_{350} = -1.415\ [kcal * mol^{-1}] \tag{8}$$

2.1.2 Second strand of DNA, right strand on figure 1

The computation of ΔH^* in $[kcal * mol^{-1}]$ is executed as follow :

$$\Delta H^* = 5\Delta H_{AA/TT} + 2\Delta H_{AT-term} \tag{9}$$

Using the Santalucia's parameters, the following value is obtained :

$$\Delta H^* = -34.9\ [kcal * mol^{-1}] \tag{10}$$

Then the computation of ΔS^* in $[cal * mol^{-1} * K^{-1}]$ is executed as follow :

$$\Delta S^* = 5\Delta S_{AA/TT} + 2\Delta S_{AT-term} \tag{11}$$

Using the Santalucia's parameters, the following value is obtained :

$$\Delta S^* = -102.8\ [cal * mol^{-1} * K^{-1}] \tag{12}$$

$$\Delta S^* = -0.1028\ [kcal * mol^{-1} * K^{-1}] \tag{13}$$

It has to be noted that here the symmetry correction is not used in the above computation has it is not clear, from the slides, when it should be included and what kind of symmetry we are talking about.

The computation of ΔG^* in $[kcal * mol^{-1}]$ is executed as follow :

$$\Delta G^* = \Delta H^* - T\Delta S^* \tag{14}$$

With T = 300K and the values found above $\Delta H^* = -37.5\ [kcal * mol^{-1}]$ and $\Delta S^* = -0.1031\ [kcal * mol^{-1} * K^{-1}]$:

$$\Delta G^*_{300} = -4.06\ [kcal * mol^{-1}] \tag{15}$$

With T = 350K and the values found above $\Delta H^* = -37.5\ [kcal * mol^{-1}]$ and $\Delta S^* = -0.1031\ [kcal * mol^{-1} * K^{-1}]$:

$$\Delta G^*_{350} = 1.08\ [kcal * mol^{-1}] \tag{16}$$

If the symmetry correction should be used, addtionnal $-1.4[cal * mol^{-1} * K^{-1}]$ should be included in the computation of ΔS^*, it would change the ΔG^* values.

2.2 Are these DNAs hybridized or denatured at these above conditions?

As explained during the lecture, the formation of the doubled stranded structures only happens when the $\Delta G^* < 0$. In other words, it will hybridized when $\Delta G^* < 0$ and denatured when $\Delta G^* > 0$.

2.2.1 First strand of DNA, left strand on figure 1

In this case, $\Delta G^*_{300} = -6.57\ [kcal * mol^{-1}]$ and $\Delta G^*_{350} = -1.415\ [kcal * mol^{-1}]$, at both temperature $\Delta G^* < 0$, therefore the DNAs are hybridized at both temperature.

2.2.2 Second strand of DNA, right strand on figure 1

In this case, $\Delta G^*_{300} = -4.06\ [kcal * mol^{-1}]$ and $\Delta G^*_{350} = 1.08\ [kcal * mol^{-1}]$. This DNAs strands are hybridized at T = 300 K but denatured at T = 350 K.

The DNAs on the right of figure 1 becomes denatured at 350 K because in this case, the temperature increases and combines to the randomness of the structures. The reaction is not anymore spontaneous and both brands of DNA stay apart from each other.

3 Assignment 2 : How do you think the DNA nanotechnology will advance in the future? What could be the closest output to industries? Please state your opinion.

I think that DNA nanotechnology is a promising field for the future. Indeed, the molecular structure of DNA was first identified by Francis Crick and James Watson in 1953 and it has only been understood and decoded recently. Still, with this newly discovered macromolecule, researchers have found astonishing properties. It is now possible to build DNA logic gates, nanostructures, sensors or even actuators. This shows that DNA, even in a short amount of time, was able to produce a lot of nanoscale structures and applications. Also, DNA is a very biocompatible structure, it can be replicated easily (through the cell itself) so it is highly abundant and it can be very compact. On top of that, humans have always been concerned about their health, the way to cure diseases. With the improvement of the knowledge the experts or institutes understood more about the mechanism hidden behind diseases and many of them are related to the DNA : genetic disorders, cancers (caused by DNA mutations), lacks of proteins, ect., by mastering DNA nanotechnologies, there could be new ways to cure those diseases. For all those reasons DNA nanotechnologies seems to have a great future.

The closest output to the industries would be in the medical sector such as pharmaceuticals, for drug delivery using DNA, repairing damaged DNA, sensors compounds for medical diagnostics. It could even be possible to imagine small DNA robotics for medical purposes.

4 Conclusion

In the first part of this report, the thermodynamic properties of several DNA strands where computed to establish if those would be in their hybridized or denatured state at several temperatures. Finally, the second part was dedicated to talk about the future perspectives in the DNA nanotechnology field and the possible output to the industry of such systems.

References

[1] Onoe Hiroaki & Takahashi Hidetoshi's slides of "biomimetic micro/nano engineering" course. Course #5, slide #11.

[2] Onoe Hiroaki & Takahashi Hidetoshi's slides of "biomimetic micro/nano engineering" course. Course #5, slide #28.