Computer Analysis of Base Pairing Free-Energy between Shine-Dalgarno Sequence and 16S rRNA in Various Procaryotes

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1 Introduction

It is well accepted that the 3' end of 16S rRNA is directly involved in the procaryotic translation initiation by pairing with the Shine-Dalgarno (SD) sequence, which is located in the ribosome-binding site of mRNA. According to the Shine and Dalgarno, *E. coli*'s 5'UTR has the pattern of "AGGAG" (SD sequence), which is complement of 16S rRNA's 3' end sequence [1]. However, not all 5'UTRs of *E. coli* have this pattern.

In this work, we systematically calculated free-energy values of the base pairing between the 3' end of 16S rRNA and the 5' UTR of mRNA, in order to detect the mRNA binding sequence in 16S rRNA for various procaryotes.

2 Materials and Methods

With window gauge of 20bps, we exhaustively compute free energy values of base pairing of 5'UTR sequence of each gene with the 3' end sequence of 16S rRNA, using parameters based on thermodynamic studies [2].

In this way, free-energy value is computed for each base position of each gene. We then take average of those free-energy values for each base position, and plotted them to visualize base-pairing patterns of the whole genome.

3 Results and discussion

The average free-energy values sharply drop about 15 bps upstream of the start codon in *E. coli*, which is consistent with the model that the 3' end of 16S rRNA interacts with the SD sequence. *H. influenzae* and *B. subtilis* shows quite a similar pattern, indicating that the organisms have basically the same translation initiation mechanism (Fig. 1).

Other species, such as *M. genitalium*, *M. pneumoniae*, *B. burgdorferi*, *H. pylori* and *Synechocystis PCC6803*, also show free-energy drops, although the drops are less evident (Fig. 2) and the shapes of the drops is significantly different from those in Fig. 1.

No free-energy drops can be seen in the genomes of *Aquifex aeolicus* and three archibacteria, *M. jannaschii*, *M. thermoautotrophicum* and *A. fulgidus* (Fig. 3), suggesting that 16S rRNA of those procaryotes does not base pair with a specific region of mRNA. Those results lead us to suspect that these procaryotes employ an alternative mechanism for translation initiation.

Acknowledgements

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References

[1] Shine, J. and Dalgarno, L., The 3'-terminal sequence of Escherichia coli 16S ribosomal RNA:Complementarity to nonsense triplets and ribosome binding sites, *Proc. Nat. Acad. Sci. USA*, 71:1342–1346, 1974.

[2] Turner, D.H. et al., Improved parameters for prediction of RNA structure, *Cold Spring Harb. Symp. Quant. Biol.*, 52:123–133, 1987.

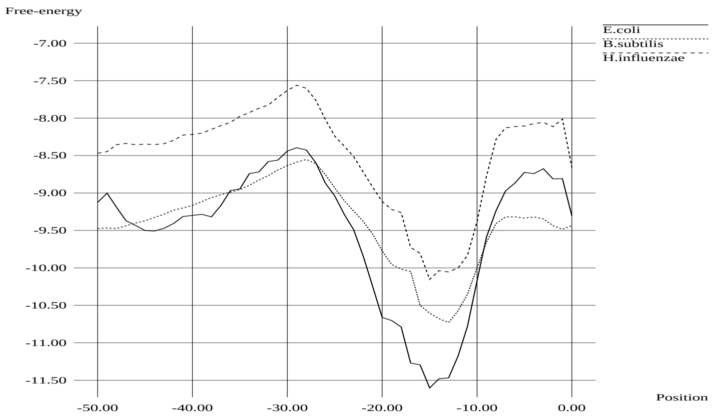

Figure 1: Sharp drops in free-energy values.

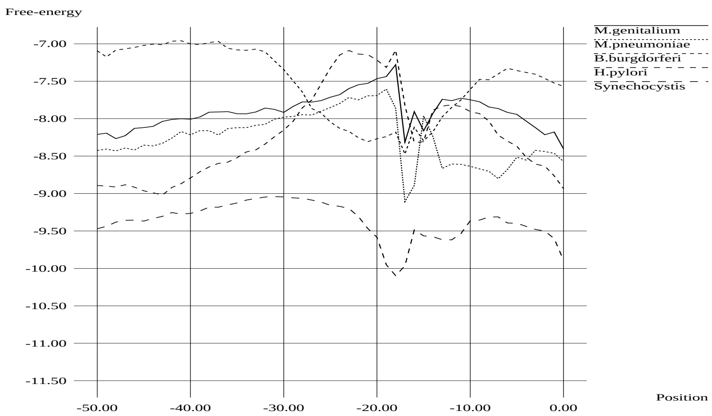

Figure 2: Less evident drops.

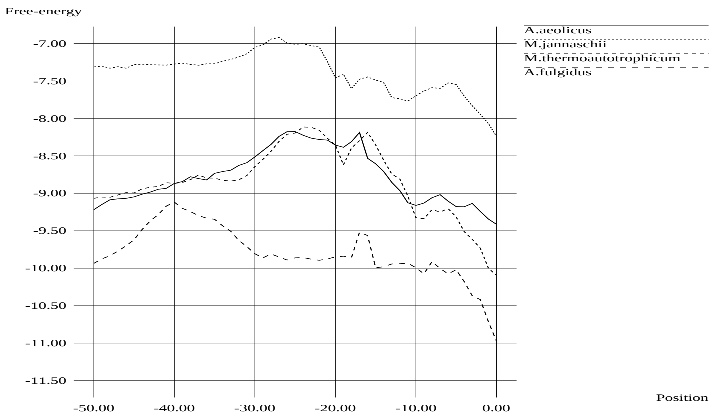

Figure 3: No significant drops.