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Robustness Criteria of Hybridization of double-stranded DNA Sequences

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Predicting the behavior of DNA molecules in vitro is a fundamental issue on DNA computing and related areas, but is also known to be quite difficult. Computational simulation is one of the most reasonable approaches for the prediction, which enables us to circumvent money/time-consuming biochemical experiments, and several simulation models have been proposed indeed. However, simulation approaches are still time-consuming in some scenario; for example, in order to design DNA sequences that hybridize in some preferable way, standard local search algorithms need to refer thousands of simulation results, which is actually impossible to complete it in reasonable computational time. In this paper, we propose simple criteria that are useful to roughly predict the behavior of DNA sequence hybridization. By using this criteria, we can determine whether a given DNA sequence *s* and its complement sequence *s'* form the perfect double stranded structures quickly, or slowly. The proposed criteria do not require computational simulations and can be easily computed. We conducted computational experiments that simulate hybridization of double-stranded DNA sequences under a probabilistic simulation model proposed in [1], whose validity is shown via comparison with biochemical experiments. The simulation results show that the proposed criteria are promising to predict the hybridization speed of double-stranded DNA sequences.

[1] Masashi Shiozaki, Hirotaka Ono, Kunihiko Sadakane, Masafumi Yamashita: A Probabilistic Model of the DNA Conformational Change. Proceedings of DNA 2006, Lecture Notes in Computer Science, 4287 274-285, 2006.