KINETICS OF THE CONFORMATIONAL TRANSFORMATION BETWEEN B- AND A-FORMS IN A SHORT DNA MOLECULE

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Some DNA sequences in crystals and in complexes with proteins can exist in the forms intermediate between the B- and A-DNA. Based on this, it was implied that the B to A transition for any DNA molecule should go through these intermediate forms also in kinetics. More precisely, the helix parameter *Slide* has to change first, and the molecule should take the E-form. After that, the *Roll* parameter changes. In the present work [1], we simulated the kinetics of the B-A transition in the Drew-Dickerson dodecamer, a known B-philic DNA oligomer. We used the "sugar" coarse-grained model [2] that reproduces ribose flexibility, preserves sequence specificity, employs implicit water and explicit ions, and offers the possibility to vary friction. As the control parameter of the transition, we chose the volume available for a counter-ion and considered the change from a large to a small volume. In the described system, the B to A conformational transformation proved to correspond to a first-order phase transition. The molecule behaves like a small cluster in the region of such a transition, jumping between the A and B forms in a wide range of available volumes [3]. The viscosity of the solvent does not affect the midpoint of the transition, but only the overall mobility of the system. All helix parameters change synchronously on average, we have not observed the sequence "*Slide* first, *Roll* later" in kinetics, and the E-DNA is not a necessary step for the transition between the B and A forms in the studied system. So, the existence of the intermediate DNA forms requires specific conditions shifting the common balance of interactions: certain nucleotide sequence in specific solution or/and the interaction with some protein.

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References

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