Calculation of Thermodynamic Parameters for Helix-to-Coil Transition in Duplex and Triplex Complexes of Oligoadenilate

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1 Introduction

Antisense and antigene drugs on the base of oligonucleotides are increasingly being considered for genetic therapy. These nucleic acid compounds could be used to repress transcription and control gene expression by the duplex or triplex formations with RNA and DNA target sites. It is known that intercalating dye being covalently attached to the terminal phosphate group of oligonucleotides stabilizes the double- and triple-helix formation. For this aim phenazole nucleoside has been attached to the 3'-end of an oligonucleotide via the ribose residue of the dye glicoside. Stabilizing effects of this modification have been studied, investigating the duplex and triplex formation of pentadecoadenilate.

2 Methods and Results

Helix-to-coil transitions in pentadecoadenilatecomplexes with decothymidylate and dodecothymidylate as well as with intercalating phenazine dye attached covalently, have been thermodynamically analyzed. At molar strand ratios 1:1 and 1:2 upon the sodium ion concentration of 0.1 and 1 M thermodynamic transition parameters (enthalpy, entropy and free energy) as well as equilibrium constants were calculated for duplex and triplex structures by the help of the two state model and the modified staggering zipper model [1]. Declination of experimental dependences from the two state model was found for duplexes containing phenazine attached. This effect is interpreted as a result of the effect of the impurity triplex state. It was stated by the help of model staggering zipper calculations that terminal group of the complexes are in a partially disordered state the degree of which increases with temperature. It is shown that strengthening of both complex types by the dye attached may be taken into account by multiplication of the complex binding constant by the attachment constant of the dye in the complementary structure.

References

[1] Blagoi, Y., Zozulya, V., and Shcherbakova, A., Thermodynamic of helix-to-coil transition in duplex and triplex complexes of oligoadenilate with oligothymidylate. Influence of covalently attached dye, *Biophysical Bulletin* (Kharkov University Bulletin, Ukraine), 1:21–32, 1998.