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NMR and Molecular Modeling Studies on the Structures of AA Mismatched DNA Oligomers

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Since the repair efficiency of non-Watson-Crick base pairs in DNA is affected by the mismatched base-pairs and their neighbor sequences, the structural studies are necessary for the elucidation of the repair efficiency. NMR and molecular modeling studies on the DNA duplexes including AA mismatches were performed. The two palindromic duplexes studied here have different nearest neighboring sequences to the mismatches: 5-d(CGACAATTGACG) ('m Ⅰ') and 5-d(CGAGAATTCACG) ('mⅡ').

Here, the structural differences of the two molecules and the existence of hydrogen-bonding between the two mismatched adenines were focused. A hydrogen bond between the mismatched adenines of 'm Ⅰ' was observed while that of 'mⅡ' was not. Though the global structures of the two molecules resemble B-form DNA, the local conformations near and at the mismatched sites are quite different from each other due to the different nearest neighboring sequences. The two mismatched adenines of 'm Ⅰ' are stacked into the helix. But, for 'mⅡ', one (A3) of the two adenines which is surrounded by the guanines is looped out of the helix and the other adenine (A10) surrounded by the cytosines is stacked into the helix. Since the looped-out bases are difficult to be repaired, the repair efficiency of 'm Ⅰ' will be better than that of 'mⅡ'.