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Silver(I)-Mediated Cytosine Self-Pairing is Preferred Over Hoogsteen-Type Base Pairs with the Artificial Nucleobase 1,3-Dideaza-6-Nitropurine

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Abstract

A 2′-deoxyribonucleoside containing 1,3-dideaza-6-nitropurine was synthesized and incorporated into oligonucleotides. The acid-base properties of this nucleoside and the corresponding N9-methylated derivative were investigated by pD-dependent ^{1}H NMR spectroscopy. A possible formation of Hoogsteen-type base pairs with cytosine was studied by ultraviolet (UV) and circular dichroism (CD) spectroscopy in the presence and absence of Ag(I) and under neutral and acidic conditions, respectively. In each case, no indication for the formation of Hoogsteen-type base pairs was obtained, which is attributed to the higher affinity of cytosine to form self-complementary hemi-

protonated base pairs under acidic conditions and metal-mediated homo base pairs in presence of Ag(I), respectively.

Keywords:

Bioinorganic chemistry | metal-mediated base pairs | cytosine | Hoogsteen | silver(I)

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