Conformational change induced by metal-ion-binding to DNA containing the artificial 1,2,4-triazole nucleoside

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Supporting Information
Figure S1: Melting curves of d(A₇X₃T₇) in the presence of various equivalents of Hg(CF₃COO)₂. One equivalent of Hg²⁺ corresponds to one Hg²⁺ per potential metal-mediated base pair in a regular double helix. The melting temperatures $T_m$ amount to 42 °C (no Hg²⁺), 40 °C (1 equiv. Hg²⁺), and 35 °C (3 equiv. Hg²⁺), respectively. Conditions: 1 µM d(A₇X₃T₇), 150 mM NaClO₄, 5 mM MOPS pH 6.8.
Figure S2: Melting temperatures of d(A7X3T7) (■: 1 μM; ○: 3 μM) and oligonucleotide C (□: 1 μM; ○: 2 μM) in the presence of various equivalents of AgNO3. In contrast to d(A7X3T7), the fluorophore-labeled oligonucleotide C shows a melting behavior indicative of hairpin formation at all given silver(I) concentrations (i.e. its $T_m$ is independent of both silver(I) and oligonucleotide concentration). Conditions: 150 mM NaClO4, 5 mM MOPS pH 6.8.
Figure S3: CD spectra of d(A7X3T7) in the presence of various equivalents of AgNO3. One equivalent of Ag⁺ corresponds to one Ag⁺ per potential metal-mediated base pair in a regular double helix. Conditions: 6.4 µM d(A7X3T7), 150 mM NaClO₄, 5 mM MOPS pH 6.8.
Figure S4: UV spectrum of 1,2,4-triazole nucleoside in H$_2$O. Conditions: 32 mM nucleoside.
Figure S5: MALDI-TOF spectra of d(A7X3T7) with different equivalents of silver(I). As can be seen from the increase in peak intensity, the addition of silver(I) leads to a stabilization of the double helical conformation.