Electronic Supplementary Information (ESI)

The Effect of the Adenine Moiety on the DNA Minor Groove-Binding of copper(II) Terpyridine complex

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Fig. S1 The ESI MS spectra of complexes 1 and 2.

(A) ESI-MS spectrum of complex 1 in water

(B) ESI-MS spectrum of complex 2 in CH₃CN
Fig. S2 Electronic absorption spectra of atpy, ttpy, complexes 1 and 2 at ambient temperature in dry, degassed CH$_3$CN

![Spectra graph]

Figure S3 RMS deviation of DNA backbone with respect to the first structures in the simulation of complexes 1 (a) and 2 (b) bound to an oligonucleotide duplex 5'-CACA$_4$A$_5$AATGT-3'/3'-GTGTTTTACA-5' and the potential energy of complexes 1 (c) and 2 (d).

![RMS deviation graphs]

Figure S4 Views of the rotation of the complex 1 in the minor groove of an oligonucleotide duplex 5'-CACA$_4$A$_5$AATGT-3'/3'-GTG$_{14}T_{15}$TTACA-5' driven by the backward reversal of the adeninyl moiety. The green and red strands represent 5'-CACA$_4$A$_5$AATGT-3' and 3'-GTG$_{14}T_{15}$TTACA-5', respectively, A$_4$ was labeled in orange while T$_{14}T_{15}$ were labeled in blue.

![Rotation views]
Effect of adenine moiety on DNA binding property of copper(II)-Terpyridine complexes

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