

## Supplementary Information

### Probing the B-to-Z-DNA Duplex Transition Using Terminally Stacking Ethyne Pyrene-Modified Adenosine and Uridine Bases

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**Table S1.** MALDI-TOF Mass Spectral Data for the ODNs [ $M^+$ ]

Sequence	Calcd $m/z$	Found $m/z$
<b>A1</b>	3278	3275
<b>U1</b>	3215	3214
<b>N1</b>	2741	2742
<b>N2</b>	2701	2669

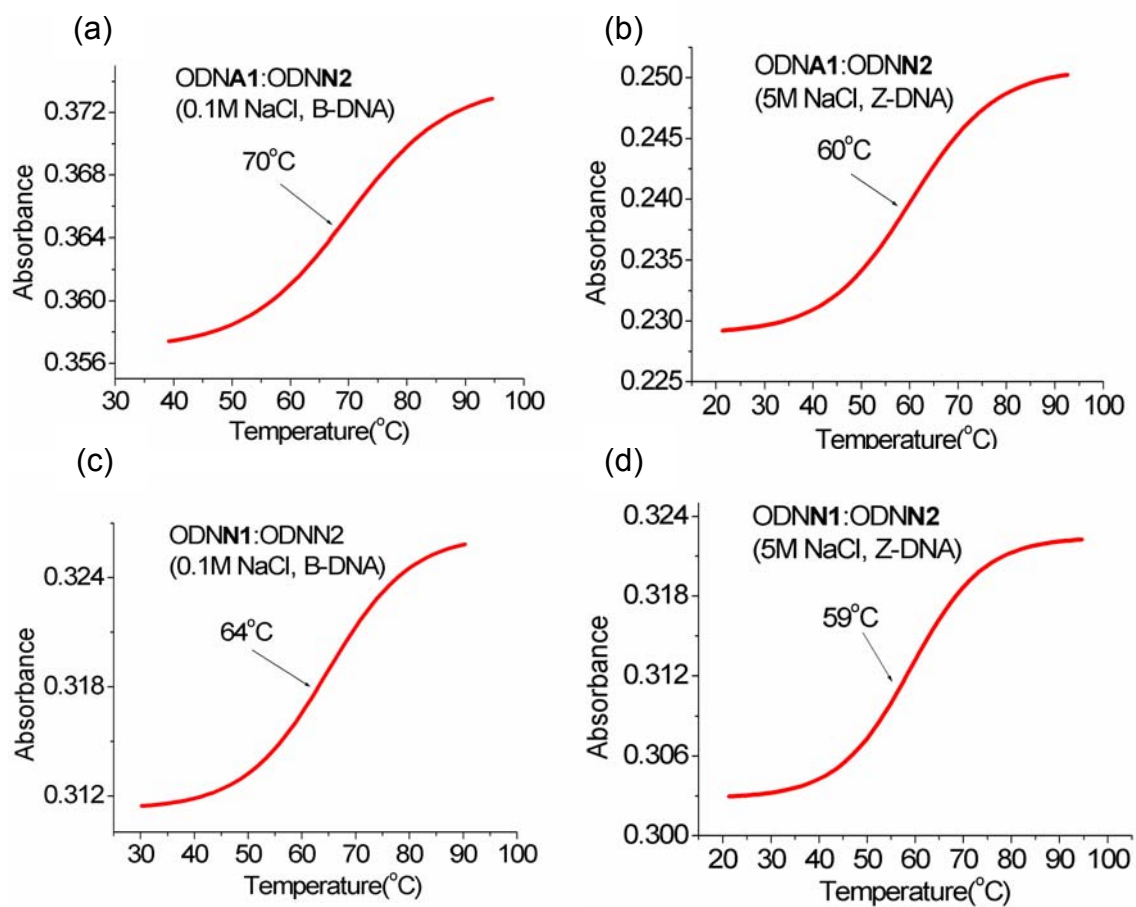


Figure S1. Melting temperature spectra of the A1·N2 and N1·N2 duplexes. The spectra were recorded at 20 °C in a buffer of 100 mM Tris-HCl (pH 7.2). Each ODN concentration was 1.5  $\mu$ M and the absorption wavelength was 260 nm.

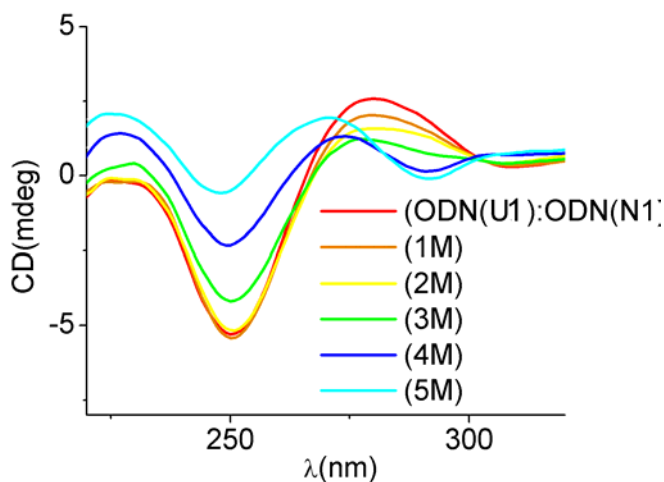


Figure S2. Circular dichroism spectra of the **U1·N1** duplex. The spectra were recorded at 20 °C in a buffer of 100 mM Tris-HCl (pH 7.2) after successively increasing the concentration of NaCl. Each ODN concentration was 1.5  $\mu$ M and the absorption wavelength was 260 nm.

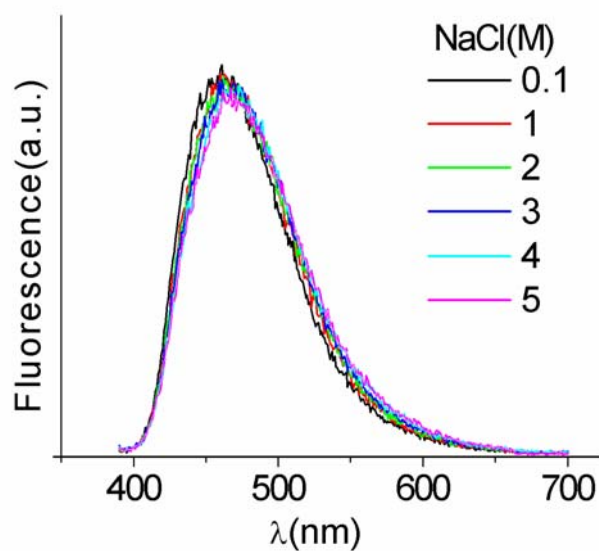


Figure S3. Fluorescence spectra of the single-stranded oligodeoxyadenylate **C1** (5'-A<sup>PY</sup> AAG TCG CAC) at various NaCl salt concentrations. These spectra were recorded at 20 °C in a buffer of 100 mM Tris-HCl (pH 7.2) at 386 nm.

This is a control experiment only to know the salt effect of the fluorophore. From this data, we know that our fluorophore material is not affected by alternating salt concentration. Therefore, it is confirmed that the fluorescence signal change of our system must be due to a B to Z conformational change of the DNA.