Supplementary Information

Probing the B-to-Z-DNA Duplex Transition Using Terminally Stacking Ethynyl Pyrene-Modified Adenosine and Uridine Bases
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Table S1. MALDI-TOF mass spectral data for the ODNs.

Figure S1. Melting temperature spectra of the A1·N2 and N1·N2 duplexes.

Figure S2. Circular dichroism spectra of the U1·N1.

Figure S3. Fluorescence spectra of ODN C1 at various NaCl concentrations.
Table S1. MALDI-TOF Mass Spectral Data for the ODNs [M$^+$]

<table>
<thead>
<tr>
<th>Sequence</th>
<th>Calcd m/z</th>
<th>Found m/z</th>
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<tbody>
<tr>
<td>A1</td>
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<td>3275</td>
</tr>
<tr>
<td>U1</td>
<td>3215</td>
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<tr>
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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 µM 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 µM and the absorption wavelength was 260 nm.

Figure S3. Fluorescence spectra of the single-stranded oligodeoxyadenylate C1 (5'-A<sup>TPY</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 control experiment only to know the salt effect of fluorophore. From this data we know that our fluorophore material is not affected on alternating salt concentration. Therefore it is confirmed that the fluorescence signal change of our system must be due to B to Z conformational change of the DNA.