Electronic supporting information to

Investigation on the binding modes between AIE-active molecules and dsDNA by single molecule force spectroscopy

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More typical force-extension curves of DNA obtained in the presence of different concentration of AIE-active molecules. For comparison, the curves were normalized and superposed, respectively.

\textbf{trans-TPEDPy}

\textbf{cis-TPEDPy}
Fig. S1 Typical stretching curves of DNA molecules (TPEDPy and DSAI) in the presence of (A) 0.5 µM, (B) 2.0 µM and (C) 4.0 µM of AIE small molecules.

Statistical analysis on the contour length and persistence length distributions of dsDNA in the presence of different concentration of AIE molecules

Fig. S2 Contour length distributions of dsDNA (A) in the absence and (B-J) in the presence of 0.5 µM (B-D), 2.0 µM (E-G) and 4.0 µM (H-J) of trans-TPEDPy, cis-TPEDPy and DSAI, respectively.
Fig. S3 Persistence length distributions of dsDNA (A) in the absence and (B-J) in the presence of 0.5 µM (B-D), 2.0 µM (E-G) and 4.0 µM (H-J) of trans-TPEDPy, cis-TPEDPy and DSAI, respectively.

Table S1 Summary of the effects of AIE molecule on the contour length and persistence length of DNA

<table>
<thead>
<tr>
<th>DNA-binding AIE molecules</th>
<th>Contour length (Lc/µm)</th>
<th>Persistence length (Lp/µm)</th>
<th>Sample size</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pure DNA</td>
<td>481.1±7.3</td>
<td>49.2±0.4</td>
<td>84</td>
</tr>
<tr>
<td>Trans-TPEDPy (µM)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.5</td>
<td>496.5±5.3</td>
<td>47.3±0.4</td>
<td>78</td>
</tr>
<tr>
<td>2.0</td>
<td>536.4±11.9</td>
<td>43.5±0.2</td>
<td>79</td>
</tr>
<tr>
<td>4.0</td>
<td>560.2±4.9</td>
<td>42.7±0.4</td>
<td>68</td>
</tr>
<tr>
<td>Cis-TPEDPy (µM)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.5</td>
<td>485.1±7.5</td>
<td>44.3±0.4</td>
<td>114</td>
</tr>
<tr>
<td>2.0</td>
<td>538.1±6.9</td>
<td>38.0±0.5</td>
<td>121</td>
</tr>
<tr>
<td>4.0</td>
<td>620.7±13.8</td>
<td>27.9±0.4</td>
<td>73</td>
</tr>
<tr>
<td>DSAI (µM)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.5</td>
<td>529.3±13.2</td>
<td>45.8±0.5</td>
<td>74</td>
</tr>
<tr>
<td>2.0</td>
<td>617.0±15.3</td>
<td>43.0±0.4</td>
<td>54</td>
</tr>
<tr>
<td>4.0</td>
<td>702.5±10.8</td>
<td>40.2±0.3</td>
<td>52</td>
</tr>
</tbody>
</table>
Fig. S4 (A) Typical stretching curves of DNA molecules in the presence of different concentrations of DSABr-C6. The inset shows the normalized result, (B) The distribution of DNA persistence length in the presence of DSABr-C6.

**Effect of ionic strength on the contour length and persistence length of DNA-AIE molecule complexes**
Fig. S5 Contour length distributions of DNA in the presence of 0.5 µM (A) trans-TPEDPy, (B) cis-TPEDPy and (C) DSAI in buffer solutions with different ionic strength, respectively.
Fig. S6 Persistence length distributions of DNA in the presence of 0.5 µM (A) trans-TPEDPy, (B) cis-TPEDPy and (C) DSAI in buffer solutions with different ionic strength, respectively.

Table S2 Summary of the effects of ionic strength on the contour length and persistence length of DNA in the presence of 0.5µM AIE molecules

<table>
<thead>
<tr>
<th>Ionic strength</th>
<th>Contour length (Lc/nm)</th>
<th>Persistence length (lp/nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tris 100 mM KCl</td>
<td>Trans-TPEDPy</td>
<td>cis-TPEDPy</td>
</tr>
<tr>
<td>10 mM Tris 100 mM KCl</td>
<td>498.5 ± 5.3</td>
<td>485.1 ± 7.5</td>
</tr>
<tr>
<td>5 mM Tris 100 mM KCl</td>
<td>517.2 ± 11.0</td>
<td>491.2 ± 4.7</td>
</tr>
<tr>
<td>5 mM Tris 50 mM KCl</td>
<td>547.5 ± 11.4</td>
<td>—</td>
</tr>
<tr>
<td>10 mM Tris 100 mM KCl</td>
<td>599.7 ± 12.6</td>
<td>690.8 ± 42.3</td>
</tr>
</tbody>
</table>

Effects of salt concentration and waiting time on the dissociation of AIE molecules from DNA (more representative curves)

Fig. S7 Typical force-extension curves of DNA-AIE molecule complexes in AIE-molecule free buffer solution. (A-C) 10 mM Tris-HCl, 100 mM KCl; (D, E) 5 mM Tris-HCl, 50 mM KCl with different incubation time.
Effect of ionic strength on the CD spectra of dsDNA-TPEDPy complexes

Fig. S8 CD spectra of dsDNA in the presence of (A) trans-TPEDPy, (B) cis-TPEDPy at various ionic strength. The ratio of DNA (base pairs) to small molecule was 9.6:1.