Supplementary Material

for the manuscript entitled

Sulfonated Ni(II)porphyrin improves the detection of Z-DNA in condensed and non-condensed BZB DNA sequences.

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Materials. Oligodeoxynucleotides were purchased from AlphaDNA, the anionic Nickel(II) porphyrin (**NiTPPS**) from Frontier Scientific, and sodium cacodylate and nickel(II) chloride from Sigma-Aldrich. All solutions were prepared using ultrapure water with a resistivity of 18.2 MΩ·cm obtained from Milli-Q system. Oligonucleotides were dissolved in a sodium cacodylate buffer (1 mM, pH 7.0), annealed at 80 °C for 20 min, cooled at 1 °C/min, and kept at 4 °C. The concentration of the DNA stock solutions was quantified by UV-vis absorption spectroscopy. The concentration of ODNs is per base pair. The B- to Z-DNA transition was induced at room temperature using (a) $NiCl_2$ or (b) spermine + $NiCl_2$.

Circular Dichroism Spectroscopy. CD spectra were recorded at 20 °C using a Jasco J-815 spectropolarimeter equipped with a single position Peltier temperature control system. Conditions were as follows: scanning speed 50 nm/min, data pitch 0.5 nm, DIT 2 s, and bandwidth 1 nm. A quartz cuvette with a 1 cm path length was used for all CD experiments. Each CD spectrum was an average of at least three scans. The CD spectrum of corresponding blank was always subtracted from the CD spectrum of the sample.

UV-Vis Absorption Spectroscopy. UV-vis absorption spectra were collected at 20 °C using a Jasco V-650 or a Jasco V-530 UV-vis double beam spectrophotometer equipped with a single position Peltier temperature control system. A quartz cuvette with a 1 cm path length was used for all UV-vis experiments.

Resonance Light Scattering. Resonance light scattering data were recorded at 20 °C using a Varian Cary Eclipse fluorescence spectrophotometer equipped with a Peltier temperature control system in a synchronous scan mode. Conditions were as follows: excitation slit 2.5 nm, emission slit 2.5 nm, scan rate 600 nm/min.

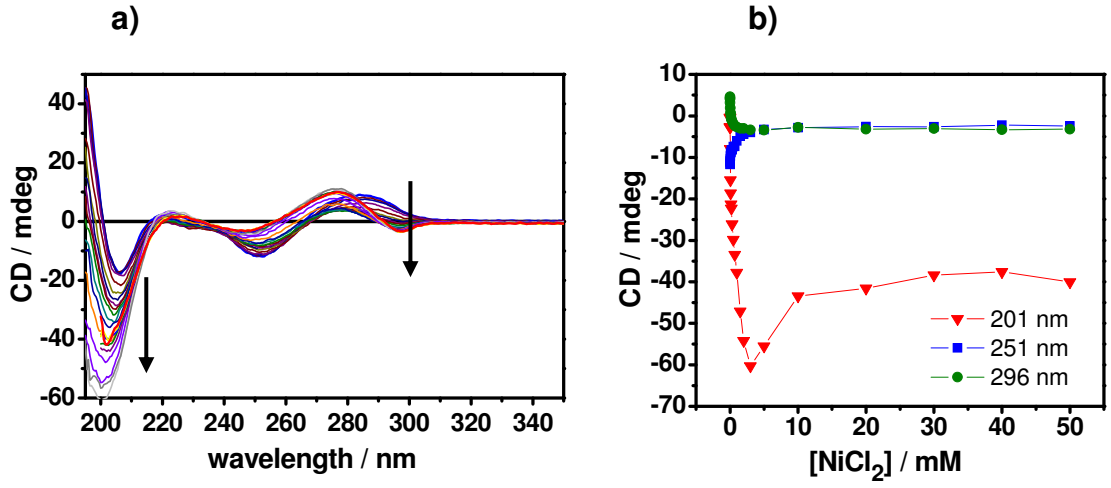

Fig. S1. a) CD spectra of $NiCl_2$ titration of **BZ** (100 μM) in Na-cacodylate buffer (1 mM, pH = 7.0). b) CD intensity at 201 nm (red triangles), 251 nm (blue squares) and 296 nm (green circles) as a function of $NiCl_2$ concentration.

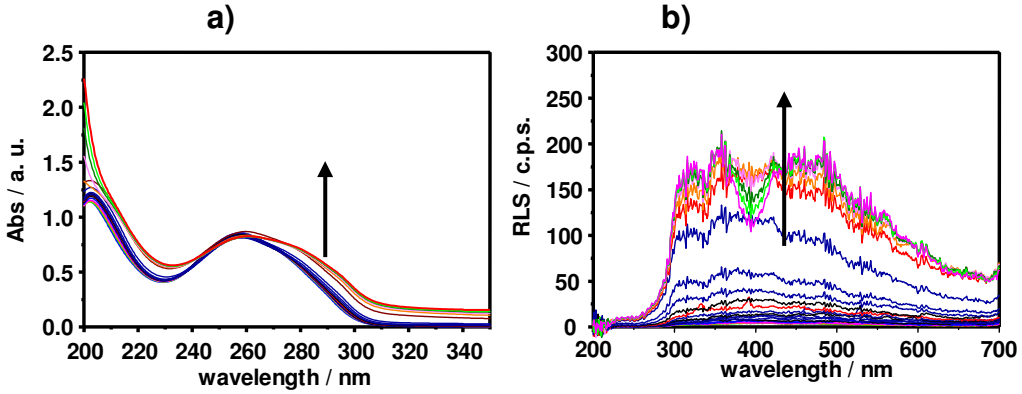

Fig. S2. a) UV and b) RLS spectra of $NiCl_2$ titration of **BZ** (100 μM) in Na-cacodylate buffer (1 mM, pH = 7.0). Arrows indicate the direction of increasing concentration of $NiCl_2$.

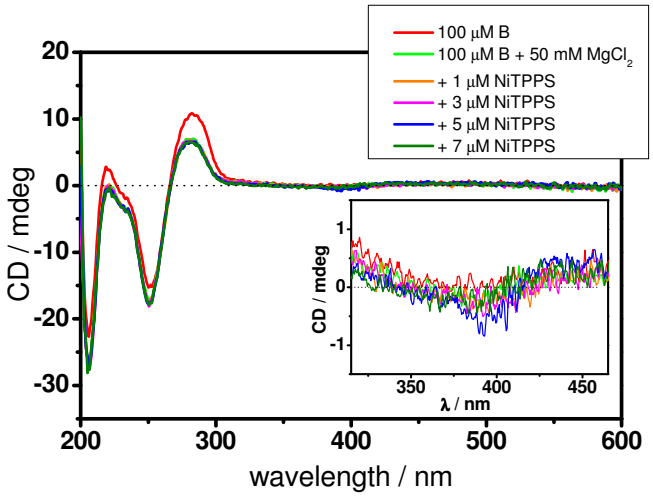

Fig. S3. CD spectra of **B** (100 μM + 50 mM $MgCl_2$) with increasing concentration of **NiTPPS**: from 1 μM to 7 μM. Inset show a zoom of ICD signal of **NiTPPS**.

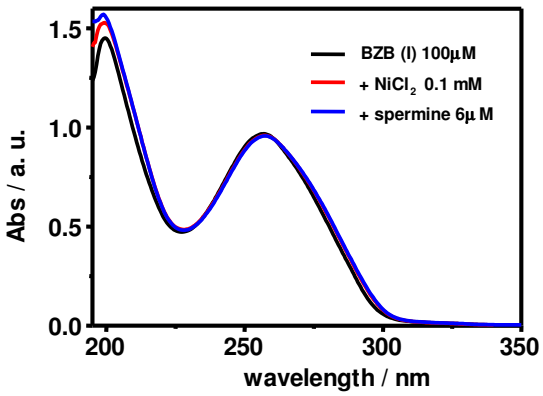

Fig. S4. UV-vis absorption spectra of **BZB(I)** (100 μM, black curve) in Na-cacodylate buffer (1 mM, pH = 7.0), in the presence of $NiCl_2$ (100 μM, red curve), and in the presence of $NiCl_2$ (100 μM) + spermine (6 μM, blue curve).

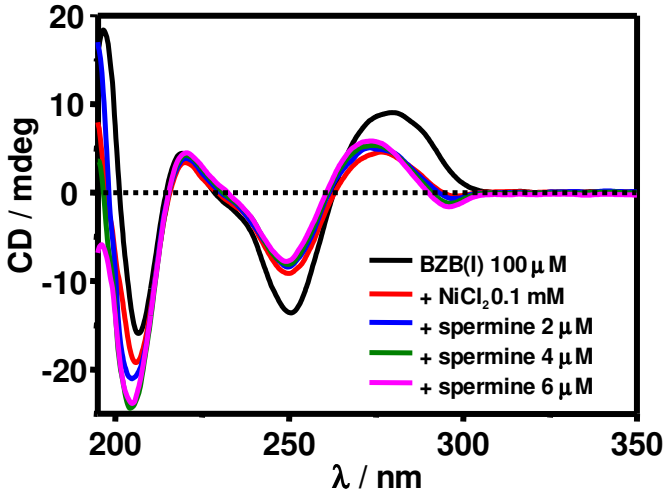

Fig. S5. CD spectra of **BZB(I)** (100 µM, black curve) in cacodylate buffer (1 mM, pH = 7.0), in the presence of $NiCl_2$ (100 µM, red curve), and $NiCl_2$ (100 µM) + spermine (from 2 µM to 6 µM).

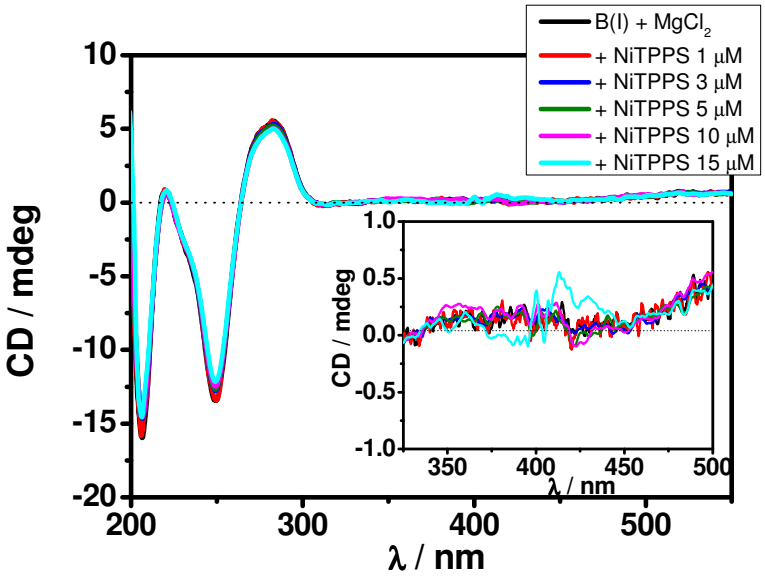

Fig. S6. CD spectra of **B(I)** (100 µM + 50 mM $MgCl_2$) with increasing concentration of **NiTPPS**: from 1 µM to 15 µM. Inset show a zoom of ICD signal of **NiTPPS**.

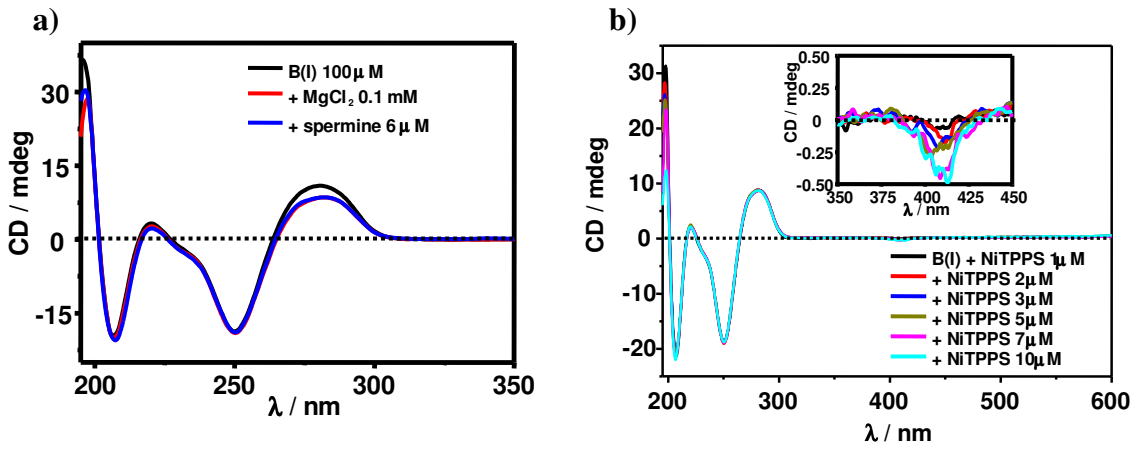

Fig. S7. a) CD spectra of **B(I)** (100 µM) in cacodylate buffer (1 mM, pH = 7.0) before (black curve), after addition of $MgCl_2$ (0.1 mM, red curve), and subsequent addition of spermine (6 µM, blue curve); b) CD spectra of **B(I)** (100 µM + 50 mM $MgCl_2$) with increasing concentration of **NiTPPS**: from 1 µM to 10 µM. Inset show a zoom of ICD signal of **NiTPPS**.

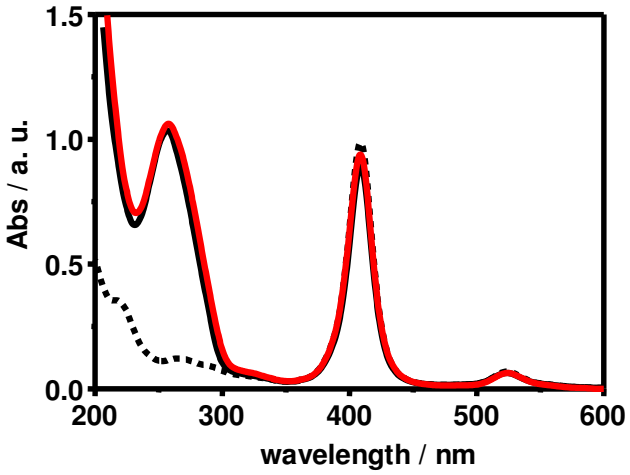

Fig. S8. UV-vis absorption spectra of **NiTPPS** (5 µM, black dashed curve) in the presence of **B(I)** (100 µM + 100 µM $MgCl_2$ + 6 µM spermine, black curve), and in the presence of **BZB(I)** (100 µM + 100 µM $NiCl_2$ + 6 µM spermine, red curve).

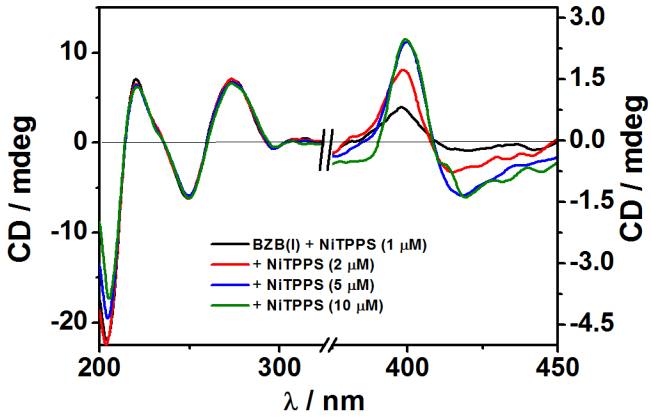

Fig. S9. CD spectra of **BZB(I)** (100 μM + 100 μM $NiCl_2$ + 6 μM spermine) in Na-cacodylate buffer (1 mM, pH = 7.0) with increasing concentration of **NiTPPS**: 1 μM (black curve), 2 μM (red curve), 5 μM (blue curve) and 10 μM (green curve).