**Supporting Information** 

for the manuscript entitled

## Porphyrin-DNA conjugates: porphyrin induced adenine-guanine homoduplex stabilization and interduplex assemblies

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**Figure S1:** HPLC chromatogram of the DNA-porphyrin conjugate **2HPor-5'a- (dAdG)**<sub>4</sub> monitored at 420 (purple) and 260 nm (blue). Inset: UV-vis absorption profile of the peak recorded by PDA detector.



Figure S2: MALDI-TOF MS of **2HPor-5'a-(dAdG)**<sub>4</sub> m/z MALDI-TOF 3149.02408 ( $C_{122}H_{124}N_{48}O_{42}P_{7'}$  [M-H]<sup>+</sup> requires 3149.72060).



**Figure S3:** HPLC chromatogram of the DNA-porphyrin conjugate **ZnPor-5'ad(dAdG)**<sub>4</sub> monitored at 425 (purple) and 260 nm (blue). Inset: UV-vis absorption profile of the peak recorded by PDA detector.



Figure S4: MALDI-TOF MS of **ZnPor-5'a-(dAdG)**<sub>4</sub> m/z MALDI-TOF 3211.04639 ( $C_{122}H_{122}N_{48}O_{42}P_7$ Zn, [M-H]<sup>+</sup> requires 3211.63410).



Figure S5: Absorption spectra of 2HPor-5'a-(dAdG)<sub>4</sub> (red curve) and ZnPor-5'a-(dAdG)<sub>4</sub> (blue curve).



Figure S6: Emission spectra of 2HPor-5'a-(dAdG)<sub>4</sub> (red curve,  $\lambda_{ex}$  = 417 nm) and ZnPor-5'a-(dAdG)<sub>4</sub> (blue curve,  $\lambda_{ex}$  = 425 nm).



**Figure S7:** HPLC chromatogram of the DNA-porphyrin conjugate **2HPor-5'p-**(**dAdG**)<sub>4</sub> monitored at 420 (purple) and 260 nm (blue). Inlet: UV-vis absorption profile of the peak recorded by PDA detector.



Figure S8: MALDI-TOF MS of **2HPor-5'p-(dAdG)**<sub>4</sub> m/z MALDI-TOF 3216.55261 ( $C_{122}H_{126}N_{47}O_{45}P_{8'}$  [M-H]<sup>+</sup> requires 3216.69168).



**Figure S9:** HPLC chromatogram of the DNA-porphyrin conjugate **ZnPor-5'p-** $(dAdG)_4$  monitored at 420 (purple) and 260 nm (blue). Inlet: UV-vis absorption profile of the peak recorded by PDA detector.



Figure S10: MALDI-TOF MS of ZnPor-5'p-(dAdG)<sub>4</sub> m/z MALDI-TOF 3279.03078 ( $C_{122}H_{124}N_{47}O_{45}P_8$  Zn, [M-H]<sup>+</sup> requires 3278.60518).



Figure S11: Absorption spectra of 2HPor-5'p-(dAdG)<sub>4</sub> (red curve) and ZnPor-5'p-(dAdG)<sub>4</sub> (blue curve).



Figure S12: Emission spectra of 2HPor-5'p-(dAdG)<sub>4</sub> (red curve,  $\lambda_{ex}$  = 417 nm) and ZnPor-5'p-(dAdG)<sub>4</sub> (blue curve,  $\lambda_{ex}$  = 425 nm).



**Figure S13:** HPLC chromatogram of the DNA-porphyrin conjugate **2HPor-5'p-** $(dGdA)_4$  monitored at 420 (purple) and 260 nm (blue). Inlet: UV-vis absorption profile of the peak recorded by PDA detector.



Figure S14: MALDI-TOF MS of **2HPor-5'p-(dGdA)**<sub>4</sub> m/z MALDI-TOF 3217.43052 ( $C_{122}H_{126}N_{47}O_{45}P_8$ , [M-H]<sup>+</sup> requires 3216.69168).



**Figure S15:** HPLC chromatogram of the DNA-porphyrin conjugate **ZnPor-5'p-**(**dGdA**)<sub>4</sub> monitored at 420 (purple) and 260 nm (blue). Inlet: UV-vis absorption profile of the peak recorded by PDA detector.



Figure S16: MALDI-TOF MS of **ZnPor-5'p-(dGdA)**<sub>4</sub> m/z MALDI-TOF 3280.70715 ( $C_{122}H_{124}N_{47}O_{45}P_8$  Zn, [M-H]<sup>+</sup> requires 3278.60518).



**Figure S17:** Absorption spectra of **2HPor-5'p-d(dGdA)**<sub>4</sub> (red curve) and **ZnPor-5'p-(dGdA)**<sub>4</sub> (blue curve).



Figure S18: Emission spectra of 2HPor-5'p-(dGdA)<sub>4</sub> (red curve,  $\lambda_{ex}$  = 417 nm) and ZnPor-5'p-(dGdA)<sub>4</sub> (blue curve,  $\lambda_{ex}$  = 425 nm).



**Figure S19:** CD spectra of **2HPor-5'a-(dAdG)**<sub>4</sub> in the absence of NaCl at -2  $^{\circ}$ C and 60  $^{\circ}$ C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S20:** UV-vis absorption spectra of **2HPor-5'a-(dAdG)**<sub>4</sub> in the absence of NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S21:** Fluorescence spectra of **2HPor-5'a-(dAdG)**<sub>4</sub> in the absence of NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Nacacodylate buffer (1 mM, pH = 7.0).



**Figure S22:** CD spectra of **2HPor-5'a-(dAdG)**<sub>4</sub> in the presence of 40 mM NaCl at -2  $^{\circ}$ C and 60  $^{\circ}$ C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S23:** UV-vis absorption spectra of **2HPor-5'a-(dAdG)**<sub>4</sub> in the presence of 40 mM NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S24:** Fluorescence spectra of **2HPor-5'a-(dAdG)**<sub>4</sub> in the presence of 40 mM NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Nacadylate buffer (1 mM, pH = 7.0).



**Figure S25:** CD spectra of **2HPor-5'a-(dAdG)**<sub>4</sub> in the presence of 100 mM NaCl. The sample was cooled from 60 °C to -2 °C at 1 °C/min. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S26**: Variable-temperature UV-vis absorption spectra of **2HPor-5'a-(dAdG)**<sub>4</sub> in the presence of 100 mM NaCl. The sample was cooled from 60 °C to -2 °C at 1 °C/min. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S27:** Variable-temperature UV-vis absorption spectra of **2HPor-5'a-(dAdG)**<sub>4</sub> in the presence of 100 mM NaCl. The sample was heated from -2  $^{\circ}$ C to 60  $^{\circ}$ C at 1  $^{\circ}$ C/min. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S28:** Fluorescence spectra of **2HPor-5'a-(dAdG)**<sub>4</sub> in the presence of 100 mM NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Nacacodylate buffer (1 mM, pH = 7.0).



**Figure S29:** CD spectra of **ZnPor-5'a-(dAdG)**<sub>4</sub> in the absence of NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] =  $5.0 \mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S30:** UV-vis absorption spectra of **ZnPor-5'a-(dAdG)**<sub>4</sub> in the absence of NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S31:** Fluorescence spectra of **ZnPor-5'a-(dAdG)**<sub>4</sub> in the absence of NaCl at -2  $^{\circ}$ C and 60  $^{\circ}$ C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S32:** CD spectra of **ZnPor-5'a-(dAdG)**<sub>4</sub> in the presence of 40 mM NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S33:** UV-vis absorption spectra of **ZnPor-5'a-(dAdG)**<sub>4</sub> in the presence of 40 mM NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S34:** Fluorescence spectra of **ZnPor-5'a-(dAdG)**<sub>4</sub> in the presence of 40 mM NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Nacadylate buffer (1 mM, pH = 7.0).



**Figure S35:** CD spectra of **ZnPor-5'a-(dAdG)**<sub>4</sub> in the presence of 100 mM NaCl. The sample was cooled from 60 °C to -2 °C at 1 °C/min. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S36:** Variable-temperature UV-vis absorption spectra of **ZnPor-5'a-(dAdG)**<sub>4</sub> in the presence of 100 mM NaCl. The sample was cooled from 60 °C to -2 °C at 1 °C/min. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S37:** Variable-temperature UV-vis absorption spectra of **ZnPor-5'a-(dAdG)**<sub>4</sub> in the presence of 100 mM NaCl. The sample was heated from -2 °C to 60 °C at 1 °C/min. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S38:** Fluorescence spectra of **ZnPor-5'a-(dAdG)**<sub>4</sub> in the presence of 100 mM NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Nacadylate buffer (1 mM, pH = 7.0).



**Figure S39:** CD spectra of **2HPor-5'p-(dAdG)**<sub>4</sub> in the absence of NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S40:** UV-vis absorption spectra of **2HPor-5'p-(dAdG)**<sub>4</sub> in the absence of NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S41:** Fluorescence spectra of **2HPor-5'p-(dAdG)**<sub>4</sub> in the absence of NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] =  $5.0 \mu$ M, Nacacodylate buffer (1 mM, pH = 7.0).



**Figure S42:** CD spectra of **2HPor-5'p-(dAdG)**<sub>4</sub> in the presence of 40 mM NaCl at - 2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S43:** UV-vis absorption spectra of **2HPor-5'p-(dAdG)**<sub>4</sub> in the presence of 40 mM NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S44:** Fluorescence spectra of **2HPor-5'p-(dAdG)**<sub>4</sub> in the presence of 40 mM NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Nacacodylate buffer (1 mM, pH = 7.0).



**Figure S45:** CD spectra of **2HPor-5'p-(dAdG)**<sub>4</sub> in the presence of 100 mM NaCl at -2  $^{\circ}$ C and 60  $^{\circ}$ C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S46:** Variable-temperature UV-vis absorption spectra of **2HPor-5'p-(dAdG)**<sub>4</sub> in the presence of 100 mM NaCl. The sample was cooled from 60 °C to -2 °C at 1 °C/min. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S47:** Fluorescence spectra of **2HPor-5'p-(dAdG)**<sub>4</sub> in the presence of 100 mM NaCl at -2  $^{\circ}$ C and 60  $^{\circ}$ C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Nacadylate buffer (1 mM, pH = 7.0).



**Figure S48:** CD spectra of **ZnPor-5'p-(dAdG)**<sub>4</sub> in the absence of NaCl at -2  $^{\circ}$ C and 60  $^{\circ}$ C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S49:** UV-vis absorption spectra of **ZnPor-5'p-(dAdG)**<sub>4</sub> in the absence of NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] =  $5.0 \mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S50:** Fluorescence spectra of **ZnPor-5'p-(dAdG)**<sub>4</sub> in the absence of NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S51:** CD spectra of **ZnPor-5'p-(dAdG)**<sub>4</sub> in the presence of 40 mM NaCl at -2  $^{\circ}$ C and 60  $^{\circ}$ C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S52:** UV-vis absorption spectra of **ZnPor-5'p-(dAdG)**<sub>4</sub> in the presence of 40 mM NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] =  $5.0 \mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S53:** Fluorescence spectra of **ZnPor-5'p-(dAdG)**<sub>4</sub> in the presence of 40 mM NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Nacacodylate buffer (1 mM, pH = 7.0).



**Figure S54:** CD spectra of **ZnPor-5'p-(dAdG)**<sub>4</sub> in the presence of 100 mM NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S55:** Variable-temperature UV-vis absorption spectra of **ZnPor-5'p-(dAdG)**<sub>4</sub> in the presence of 100 mM NaCl. The sample was cooled from 60 °C to -2 °C at 1 °C/min. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S56:** Fluorescence spectra of **ZnPor-5'p-(dAdG)**<sub>4</sub> in the presence of 100 mM NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Nacadylate buffer (1 mM, pH = 7.0).



**Figure S57:** CD spectra of **2HPor-5'p-(dGdA)**<sub>4</sub> in the absence of NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S58:** UV-vis absorption spectra of **2HPor-5'p-(dGdA)**<sub>4</sub> in the absence of NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S59:** Fluorescence spectra of **2HPor-5'p-(dGdA)**<sub>4</sub> in the absence of NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Nacacodylate buffer (1 mM, pH = 7.0).



**Figure S60:** CD spectra of **2HPor-5'p-(dGdA)**<sub>4</sub> in the presence of 40 mM NaCl at -2  $^{\circ}$ C and 60  $^{\circ}$ C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S61:** UV-vis absorption spectra of **2HPor-5'p-(dGdA)**<sub>4</sub> in the presence of 40 mM NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S62:** Fluorescence spectra of **2HPor-5'p-(dGdA)**<sub>4</sub> in the presence of 40 mM NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Nacadylate buffer (1 mM, pH = 7.0).



**Figure S63:** CD spectra of **2HPor-5'p-(dGdA)**<sub>4</sub> in the presence of 100 mM NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S64:** Variable-temperature UV-vis absorption spectra of **2HPor-5'p-(dGdA)**<sub>4</sub> in the presence of 100 mM NaCl. The sample was cooled from 60 °C to -2 °C at 1 °C/min. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S65:** Fluorescence spectra of **2HPor-5'p-(dGdA)**<sub>4</sub> in the presence of 100 mM NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Nacadylate buffer (1 mM, pH = 7.0).



**Figure S66:** CD spectra of **ZnPor-5'p-(dGdA)**<sub>4</sub> in the presence of 40 mM NaCl at -2  $^{\circ}$ C and 60  $^{\circ}$ C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S67:** UV-vis absorption spectra of **ZnPor-5'p-(dGdA)**<sub>4</sub> in the absence of NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S68:** Fluorescence spectra of **ZnPor-5'p-(dGdA)**<sub>4</sub> in the absence of NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S69:** CD spectra of **ZnPor-5'p-(dGdA)**<sub>4</sub> in the presence of 40 mM NaCl at -2  $^{\circ}$ C and 60  $^{\circ}$ C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S70:** UV-vis absorption spectra of **ZnPor-5'p-(dGdA)**<sub>4</sub> in the presence of 40 mM NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S71:** Fluorescence spectra of **ZnPor-5'p-(dGdA)**<sub>4</sub> in the presence of 40 mM NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Nacacodylate buffer (1 mM, pH = 7.0).



**Figure S72:** CD spectra of **ZnPor-5'p-(dGdA)**<sub>4</sub> in the presence of 100 mM NaCl at -2  $^{\circ}$ C and 60  $^{\circ}$ C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S73:** Variable-temperature UV-vis absorption spectra of **ZnPor-5'p-(dGdA)**<sub>4</sub> in the presence of 100 mM NaCl. The sample was cooled from 60 °C to -2 °C at 1 °C/min. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S74:** Fluorescence spectra of **ZnPor-5'p-(dGdA)**<sub>4</sub> in the presence of 100 mM NaCl at -2 °C and 60 °C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Nacacodylate buffer (1 mM, pH = 7.0).



**Figure S75:** CD spectra of **5'-(dAdG)**<sub>4</sub> in the absence of NaCl at -2 °C and 60 °C. Conditions: [DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S76:** UV-vis absorption spectra of **5'-(dAdG)**<sub>4</sub> in the absence of NaCl at -2  $^{\circ}$ C and 60  $^{\circ}$ C. Conditions: [DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S77:** CD spectra of **5'-(dAdG)**<sub>4</sub> in the presence of 40 mM NaCl at -2  $^{\circ}$ C and 60  $^{\circ}$ C. Conditions: [DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S78:** UV-vis absorption spectra of **5'-(dAdG)**<sub>4</sub> in the presence of 40 mM NaCl at -2 °C and 60 °C. Conditions: [DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S79:** CD spectra of **5'-(dAdG)**<sub>4</sub> in the presence of 100 mM NaCl at -2 °C and 60 °C. Conditions: [DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S80:** UV-vis absorption spectra of **5'-(dAdG)**<sub>4</sub> in the presence of 100 mM NaCl at -2 °C and 60 °C. Conditions: [DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S81:** CD spectra of **5'-(dGdA)**<sub>4</sub> in the absence of NaCl at -2  $^{\circ}$ C and 60  $^{\circ}$ C. Conditions: [DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S82:** UV-vis absorption spectra of **5'-(dGdA)**<sub>4</sub> in the absence of NaCl at -2  $^{\circ}$ C and 60  $^{\circ}$ C. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S83:** CD spectra of **5'-(dGdA)**<sub>4</sub> in the presence of 40 mM NaCl at -2  $^{\circ}$ C and 60  $^{\circ}$ C. Conditions: [DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S84:** UV-vis absorption spectra of **5'-(dGdA)**<sub>4</sub> in the presence of 40 mM NaCl at -2 °C and 60 °C. Conditions: [DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S85:** CD spectra of **5'-(dGdA)**<sub>4</sub> in the presence of 100 mM NaCl at -2 °C and 60 °C. Conditions: [DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S86:** UV-vis absorption spectra of 5'-(dGdA)<sub>4</sub> in the presence of 100 mM NaCl at -2 °C and 60 °C. Conditions: [DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S87:** CD spectra of six synthesized Por-DNA conjugates in the absence of NaCl at -2 °C. Conditions: [Por-DNA] =  $5.0 \mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S88:** CD spectra of **2HPor-5'a-(dAdG)**<sub>4</sub> at different concentrations in the presence of 40 mM NaCl at -2. The sample was diluted by adding a solution of Nacacodylate buffer (1 mM, pH = 7.0) with NaCl (40 mM) at -2 °C.



**Figure S89:** CD spectra of **2HPor-5'a-(dAdG)**<sub>4</sub> (5.0  $\mu$ M) at different NaCl concentration. The NaCl concentration was increased to 80 mM by addition of a stock solution (4 M). 100 mM concentration was achieved by addind solid salt. Conditions: [Por-DNA] = 5.0  $\mu$ M, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S90:** CD spectra of neat **2HPor-5'a-(AG)**<sub>4</sub> annealed from 60 °C to -2 °C (red curve); annealed from 60 °C to -2 °C with equimolar amount of 5'-(CT)<sub>4</sub> (black curve); and after addition of equimolar amount of 5'-(CT)<sub>4</sub> to preannealed **2HPor-5'a-(AG)**<sub>4</sub> at -2 °C (blue curve). Conditions: [Por-ODN] = 5.0  $\mu$ M, 100 mM NaCl, Na-cacodylate buffer (1 mM, pH = 7.0).



**Figure S91:** PAGE of **2HPor-5'a-(dAdG)**<sub>4</sub> and **2HPor-5'p-(dAdG)**<sub>4</sub>. Gel was run in Na-cacodylate buffer (1 mM, pH = 7.0) with 40 mM NaCl for 8 h at 30 mA at 0 °C. Ultraviolet lamp ( $\lambda$  = 365 nm) was used to visualize porphyrin-DNA conjugates.