

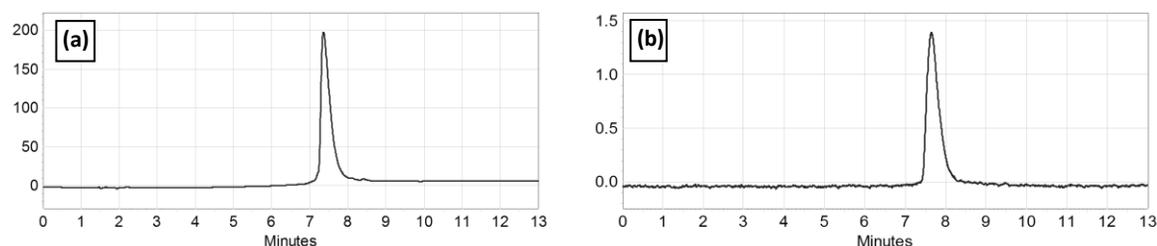
Electronic Supplementary Information

for the manuscript entitled

**Chiroptical properties, binding affinity, and photostability  
of conjugated zinc porphyrin dimer complexed with left-handed Z-DNA and  
right-handed B-DNA**

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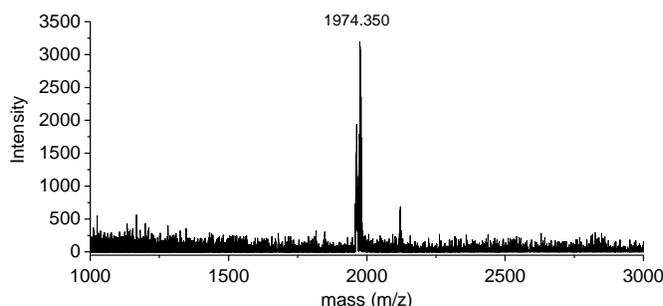


**Figure S1:** (a) Absorption ( $\lambda = 469$  nm) and (b) emission ( $\lambda_{\text{ex}} = 469$  nm,  $\lambda_{\text{em}} = 775$  nm, slit = 10 nm) HPLC chromatograms of **ZnPD**.

**Table S1:** Solvent gradient used for HPLC of **ZnPD**.<sup>‡</sup>

time/min	1% $\text{CH}_3\text{CO}_2\text{H}$ in $\text{H}_2\text{O}$	$\text{CH}_3\text{OH}$	$\text{THF}$
0	70%	25%	5%
8.0	15%	25%	60%
10.0	15%	25%	60%
11.0	70%	25%	5%
13.0	70%	25%	5%

<sup>‡</sup> Flow rate: 1 mL/min (analytical) or 4 mL/min (semi-preparative), temperature: 30 °C.



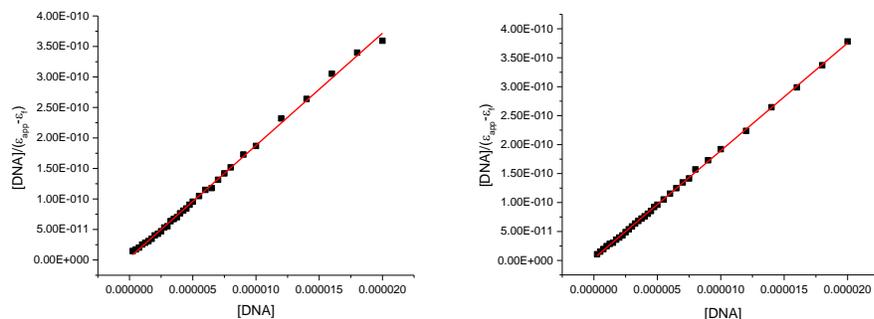
**Figure S2:** MALDI-TOF spectra of **ZnPD**.  $m/z$  1974.350 ( $\text{C}_{112}\text{H}_{106}\text{N}_{10}\text{O}_{16}\text{Zn}_2$ ,  $[\text{M}-2\text{I}]^+$ , requires 1974.636).

Binding constants of **ZnPD** with DNAs were determined by absorption spectrophotometric titration at 20 °C as previously reported.[1-5] The fixed amount of **ZnPD** ( $c = 2.24$   $\mu\text{M}$ ) in Na-cacodylate buffer (1 mM, pH = 7.0) was titrated with the stock solution of DNA ( $c = 1.80$   $\mu\text{M}$ ). The changes in absorbance of the Soret band of **ZnPD** were monitored upon addition of DNA. The apparent binding constant ( $K_{\text{app}}$ ) was calculated by the following equation:

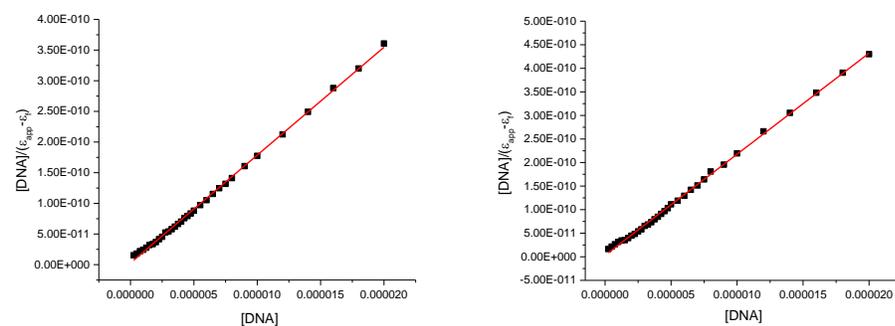
$$\frac{[\text{DNA}]_{\text{total}}}{/e_{\text{app}} - e_f/} = \frac{1}{/e_b - e_f/} [\text{DNA}]_{\text{total}} + \frac{1}{K_{\text{app}}} /e_b - e_f/$$

where  $e_{\text{app}}$  corresponds to absorbance of a given solution divided by the total ligand concentration;  $e_f$  corresponds to molar absorptivity of the free ligand;  $e_b$  corresponds to molar

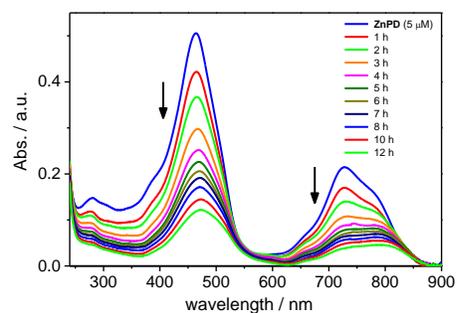
absorptivity of the total bound ligand. In the plot of  $[\text{DNA}]/(e_{\text{app}} - e_f)$  vs.  $[\text{DNA}]$ ,  $K_{\text{app}}$  is given by the ratio of the slope to the intercept.



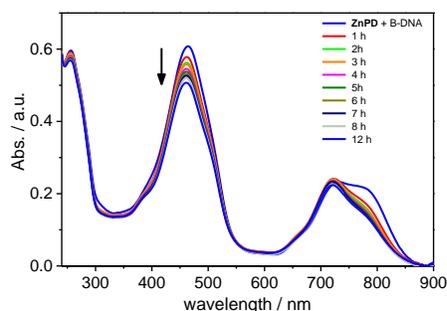
**Figure S3:** Scatchard plot of ZnPD binding with B-form of poly(dG-dC)<sub>2</sub>.  $K_{\text{app}} = 4.84 \times 10^6 \text{ M} \pm 0.23$ .



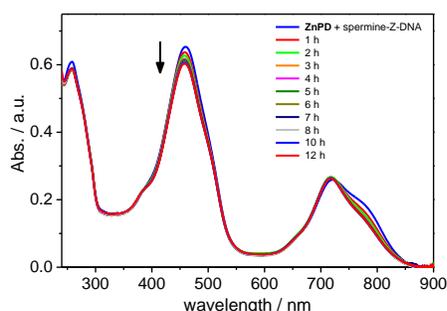
**Figure S4:** Scatchard plot of ZnPD binding with spermine-Z-poly(dG-dC)<sub>2</sub>.  $K_{\text{app}} = 6.18 \times 10^6 \text{ M} \pm 0.08$ .



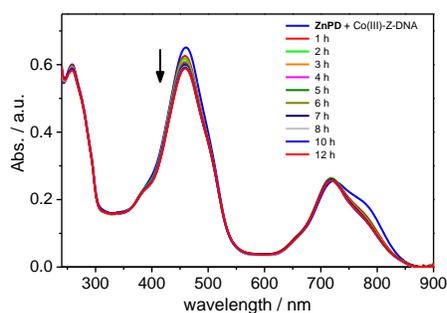
**Figure S5:** UV-vis absorption spectra of ZnPD during irradiation. Conditions:  $[\text{ZnPD}] = 5 \mu\text{M}$ , 1% DMSO Na-cacodylate buffer (1 mM, pH = 7.0, 50 mM NaCl)



**Figure S6:** UV-vis absorption spectra of **ZnPD** during irradiation in the presence of B-form of poly(dG-dC)<sub>2</sub>. Conditions: [ZnPD] = 5 μM, [poly(dG-dC)<sub>2</sub>] = 50 μM, 1% DMSO Na-cacodylate buffer (1 mM, pH = 7.0, 50 mM NaCl).



**Figure S7:** UV-vis absorption spectra of **ZnPD** during irradiation in the presence of Z-form of poly(dG-dC)<sub>2</sub> induced by spermine (12 μM). Conditions: [ZnPD] = 5 μM, [poly(dG-dC)<sub>2</sub>] = 50 μM, 1% DMSO Na-cacodylate buffer (1 mM, pH = 7.0, 50 mM NaCl).



**Figure S8:** UV-vis absorption spectra of **ZnPD** during irradiation in the presence of Z-form of poly(dG-dC)<sub>2</sub> induced by Co(III) (12 μM). Conditions: [ZnPD] = 5 μM, [poly(dG-dC)<sub>2</sub>] = 50 μM, 1% DMSO Na-cacodylate buffer (1 mM, pH = 7.0, 50 mM NaCl).

### **References:**

- [1] J.D. McGhee, P.H.V. Hippel, *J. Mol. Biol.* 1974, **86**, 469–489.
- [2] T. Yamamoto, D.H. Tjahjono, N. Yoshioka, H. Inoue, *Bull. Chem. Soc. Jpn.* 2003, **76**, 1947–1955.
- [3] R.F. Pasternack, E.J. Gibbs, J.J. Villafranca, *Biochemistry* 1983, **22**, 2406–2414.
- [4] T. Ohyama, H. Mita, Y. Yamamoto, *Biophys. Chem.* 2005, **113**, 53–59.
- [5] L.R. Keating, V.A. Szalai, *Biochemistry* 2004, **43**, 15891–15900.