

Supporting Information for manuscript entitled

Conjugated porphyrins as a CD reporter of the salt-induced B to Z-DNA transition

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Milan Balaz,* Benjamin C. Li, Jay D. Steinkruger, George A. Ellestad, Koji Nakanishi and Nina Berova*

Department of Chemistry, Columbia University, New York, New York 10027, USA

ndb1@columbia.edu, milan.balaz@chem.ox.ac.uk

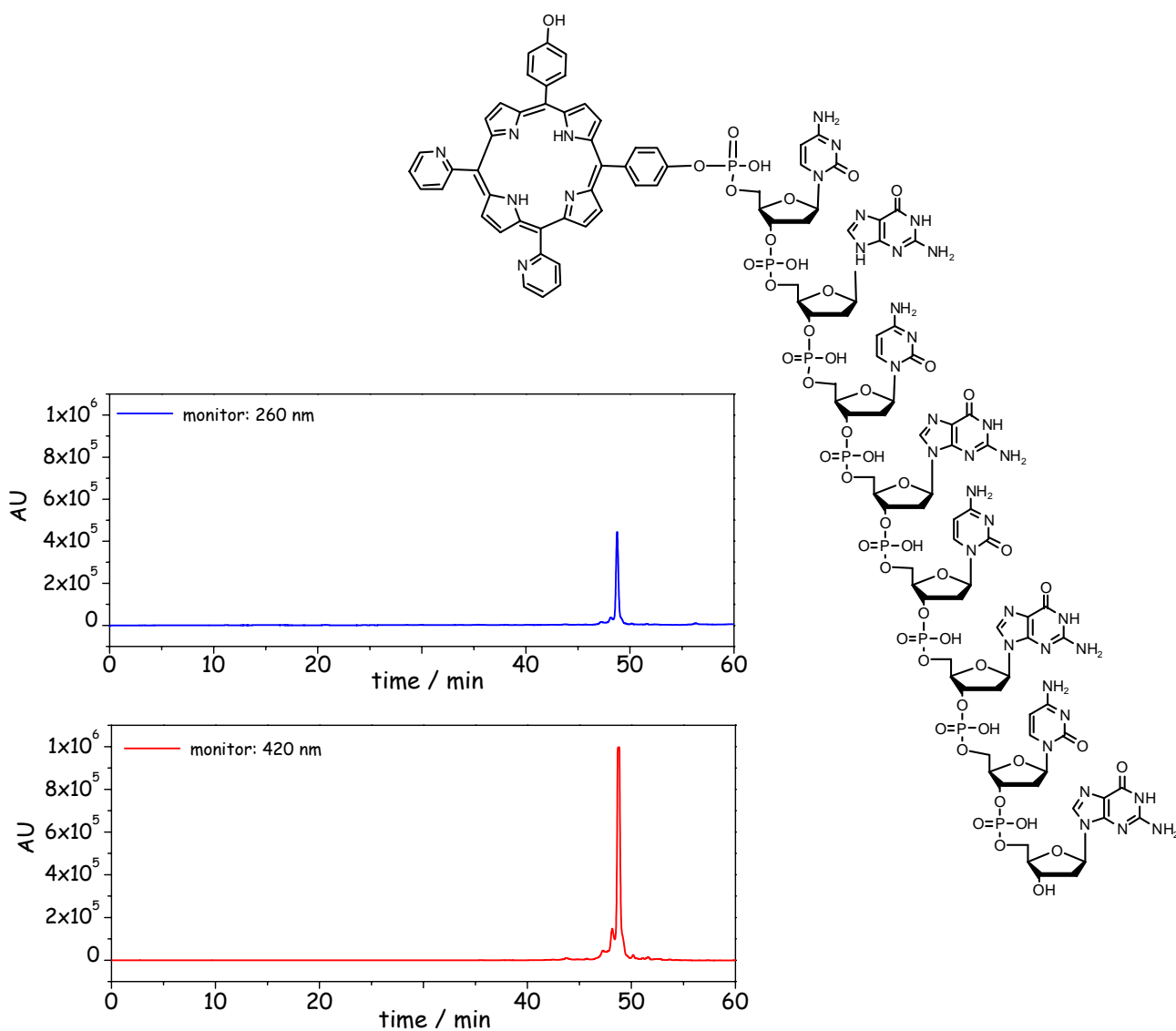
General procedures

All the measurements have been made at room temperature in 50 mM potassium phosphate buffer at pH=7.0. The concentration of the ODNs was 10^{-5} to 10^{-6} M according to the experimental details. Circular dichroism spectra were recorded on a JASCO J-810 spectrophotometer using quartz cuvettes with an optic path of 1 cm. Fluorescence emission spectra were recorded on a SPEX Fluorolog-3 spectrometer FL3-22 (J. Y. Horiba, Edison, NJ) at an excitation wavelength of 420 nm using quartz cuvettes with optical path length of 1x1 cm. Absorbance spectra were recorded on a JASCO V-530 spectrophotometer using quartz cuvettes with an optic path of 1 cm.

- page B HPLC purification of porphyrin-ODN conjugate **1P**
- page C Figure SI-1: absorption spectrum of **1P**
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- page D Figure SI-3: absorption spectrum of **1P** at different salt (NaCl and/or NiCl₂) concentrations
- page D Figure SI-4: circular dichroism spectrum of **1P** at different salt (NaCl and/or NiCl₂) concentrations
- page E Figure SI-5: circular dichroism spectrum of **1** at different salt (NaCl and/or NiCl₂) concentrations
- page E Figure SI-6: absorption spectrum of **1** at different salt (NaCl and/or NiCl₂) concentrations

HPLC purification of porphyrin-oligonucleotide conjugate **1P**

The porphyrin-oligonucleotide **1P** was synthesized according to previously described procedure.¹ **1P** was purified using a JASCO HPLC system using a Waters reverse phase X-Terra semi-preparative column MS C₁₈ 2.5 μ m 10x50mm equipped with a Fenomenex column heater Thermasphere TS-130.² During the HPLC, the profile was monitored by a JASCO two-channel array detector using 260 nm wavelength for oligonucleotide detection and 420 nm wavelength for porphyrin detection (see below).



¹ M. Balaz, J. D. Steinkruger, G. A. Ellestad, and N. Berova, *Org. Lett.*, 2005, **7**, 5613

² M. Balaz, A. E. Holmes, M. Benedetti, G. Proni, N. Berova, *Bioorg. Med. Chem.* 2005, **13**, 241

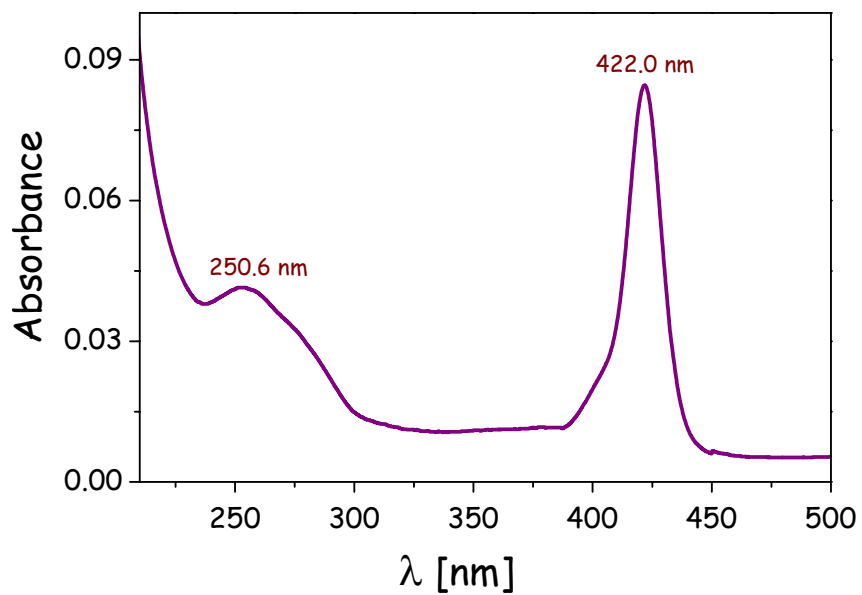


Figure SI-1. Absorbance spectra of porphyrin-ODN conjugate **1P** in 50 mM K-phosphate buffer, pH=7.0 at room temperature.

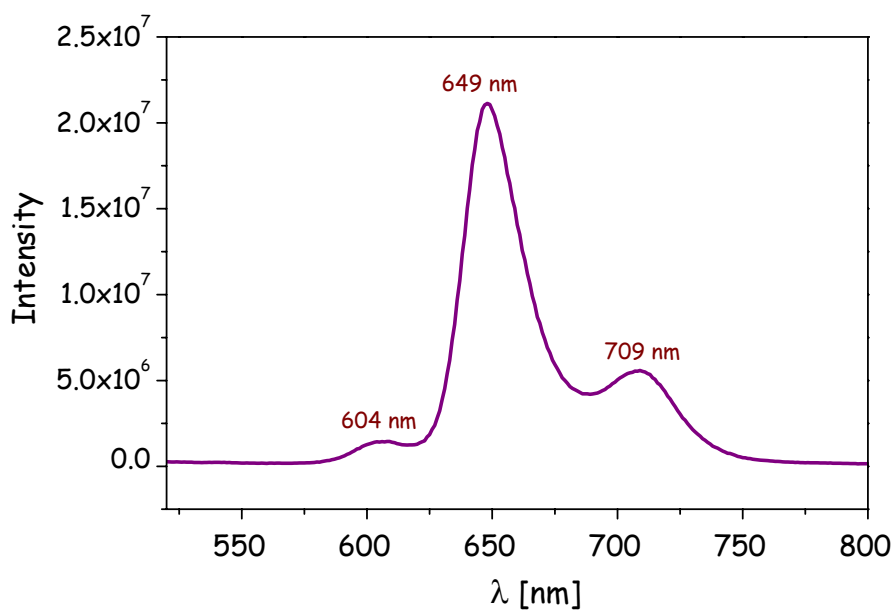


Figure SI-2. Fluorescence spectra of porphyrin-ODN conjugate **1P** in 50 mM K-phosphate buffer, pH=7.0 at room temperature.

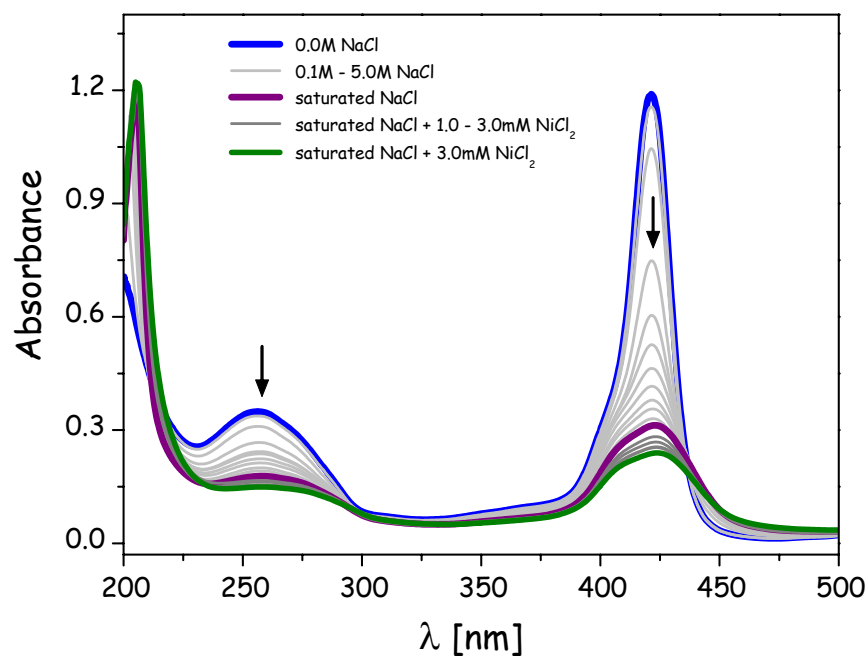


Figure SI-3 Absorption spectrum of porphyrin-8-mer conjugate **1P** at different concentration of NaCl and NiCl_2 . Conditions: 50mM K-phosphate buffer, pH=7.0; ODN concentration $\sim 5 \cdot 10^{-6}$ M.

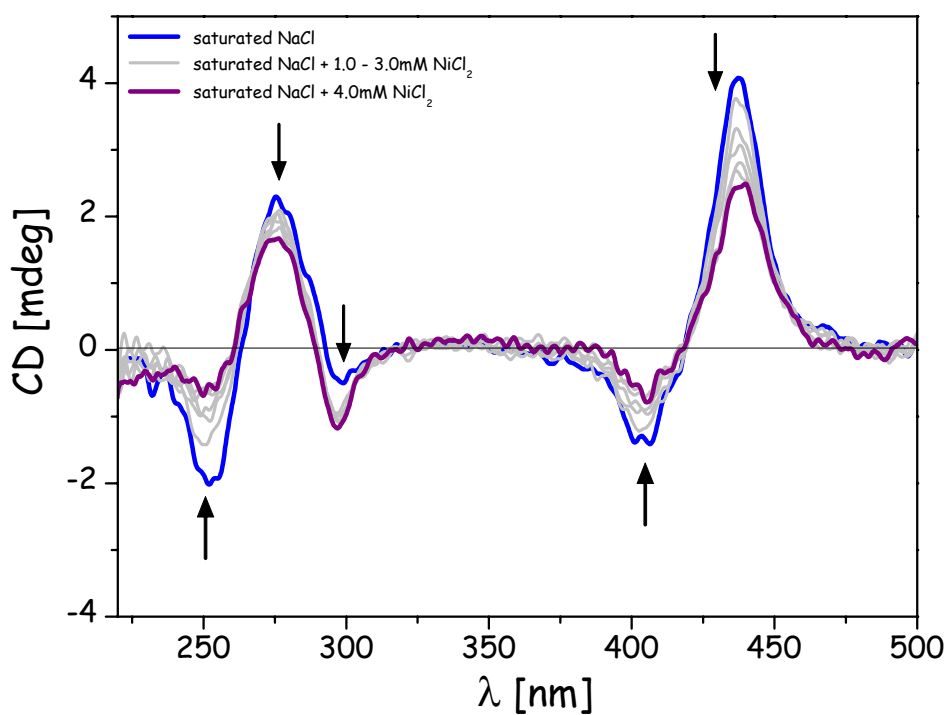


Figure SI-4 CD spectrum of porphyrin-8-mer conjugate **1P** at different concentration of NaCl and NiCl_2 . Conditions: 50mM K-phosphate buffer at pH=7.0; ODN concentration $\sim 10^{-5}$ M.

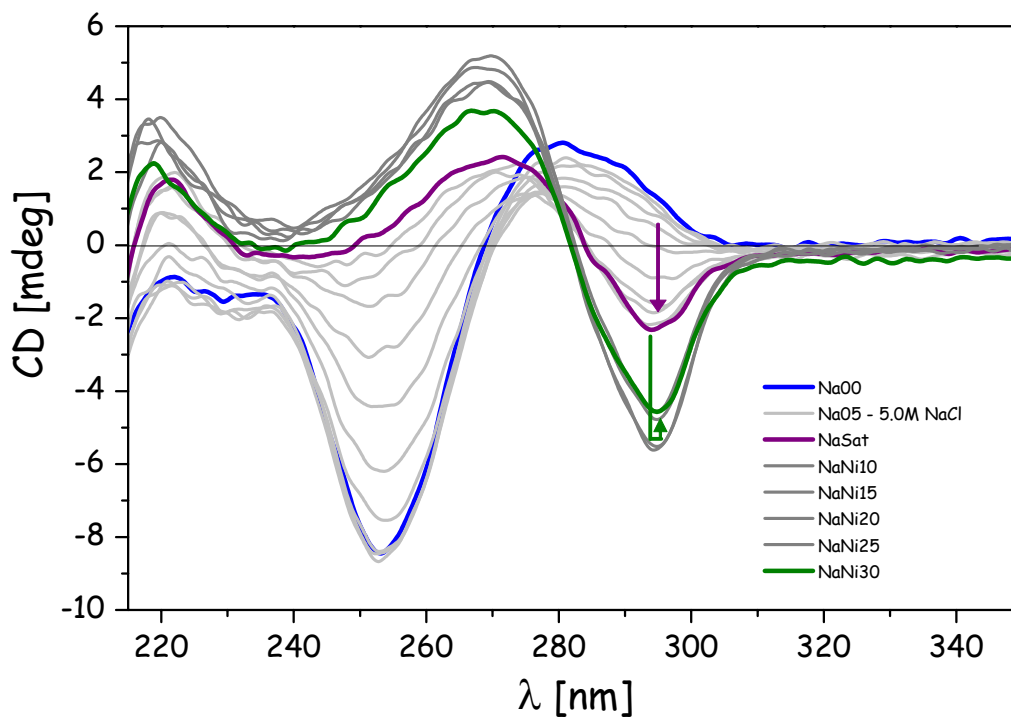


Figure SI-5 CD spectrum of 8-mer ODN **1** at different concentration of NaCl and NiCl₂.
 Conditions: 50mM K-phosphate buffer at pH=7.0.

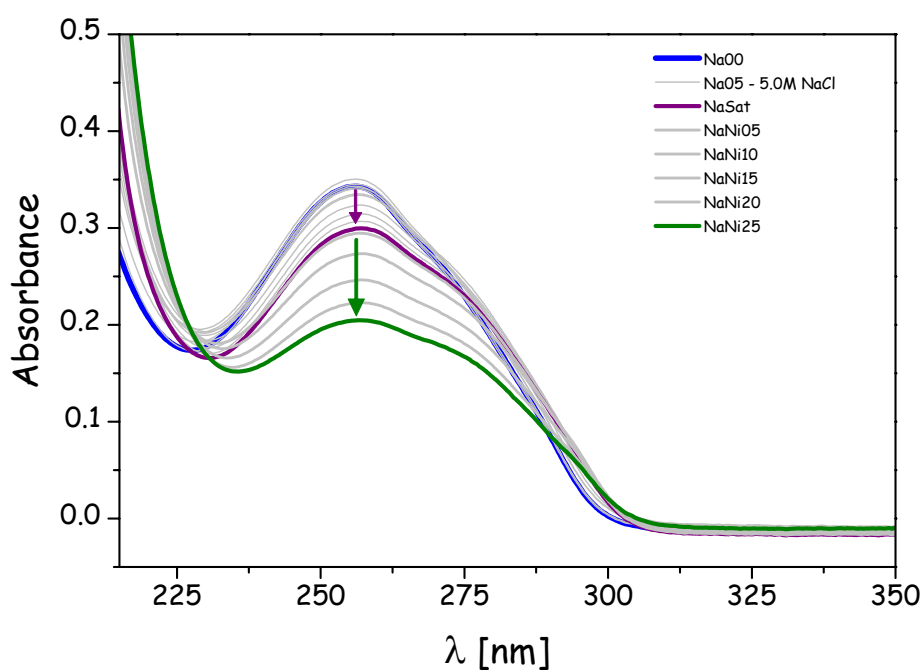


Figure SI-6 Absorption spectrum of 8-mer ODN **1** at different concentration of NaCl and NiCl₂.
 Conditions: 50mM K-phosphate buffer at pH=7.0.