Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supplementary Information

for

N-fused porphyrin with pyridinium side-arms: A new class of aromatic ligands with DNA-binding ability

Yoshiya Ikawa, Satoshi Touden, and Hiroyuki Furuta

Content:

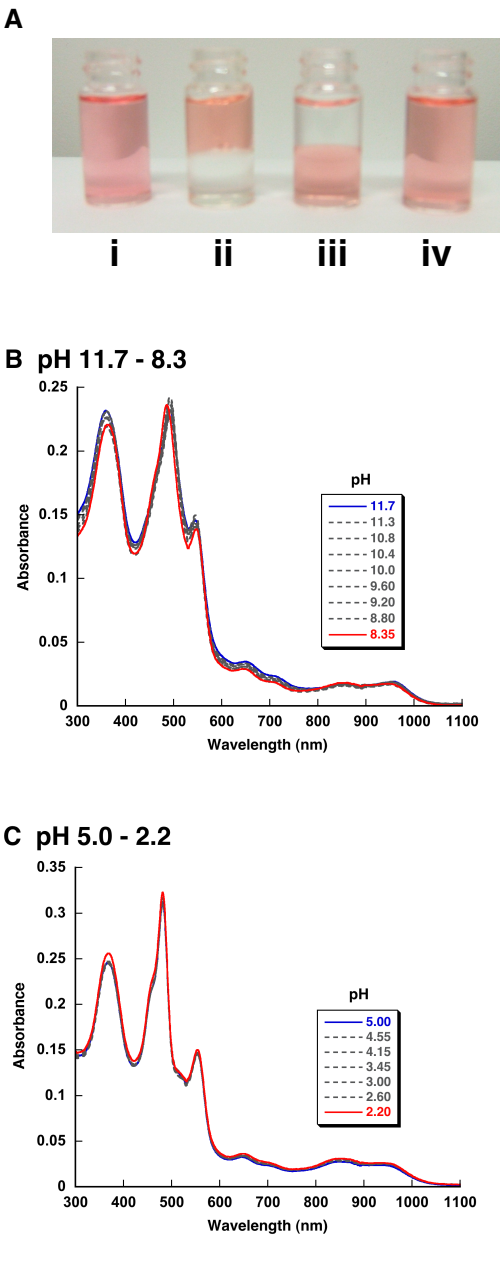


Fig. S1
Optical property of **pPyNFP** in H_2O.

A: Partition experiments of **pPyNFP** and **NFTPP**. i: **pPyNFP** in DMF, ii: **pPyNFP** in H_2O-CH_2Cl_2, iii: **NFTPP** in H_2O-CH_2Cl_2, iv: **NFTPP** in DMF.
B, C: Absorption spectra of **pPyNFP** (7.5 μM) in H_2O titrated with NaOH and HCl.
Absorption spectra for titration at pH 11.7–8.3 (B) and pH 5.0–2.2 (C).

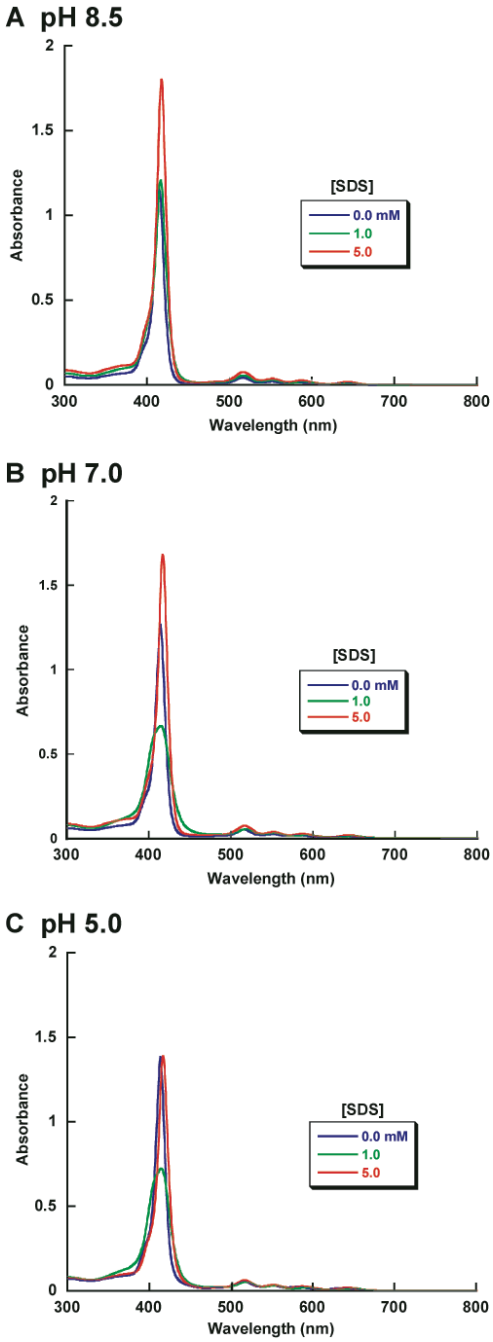


Fig. S2
UV-vis absorption spectral changes of **pPyP** (7.5 μM) by the addition of various amounts of SDS at pH 8.5 (A), 7.0 (B), and 5.0 (C).

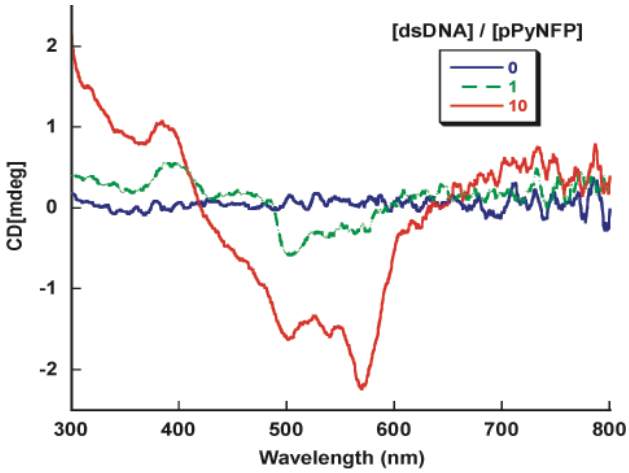


Fig. S3
Circular dichroism (CD) spectra of **pPyNFP** (7.5 μM) in the presence of the long double stranded DNA at pH 7.0 with 50 mM HEPES.

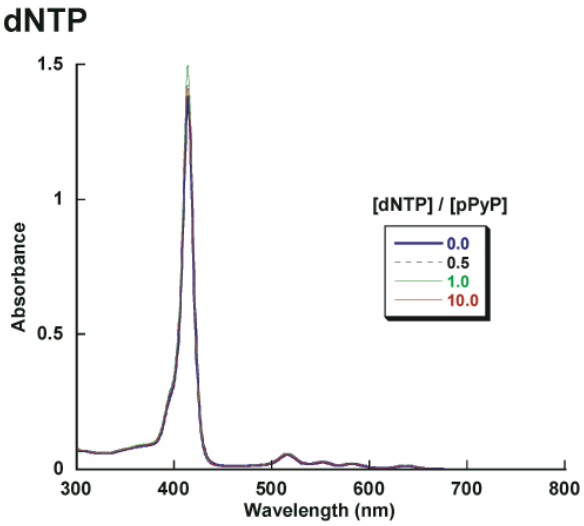


Fig. S4
Effects of deoxyribonucleotide triphosphate on **pPyP** (7.5 μM).

UV-vis absorption spectra of **pPyP** (7.5 μM) in the presence of deoxyribonucleotide triphosphate (dNTP) at pH 7.0 with 50 mM HEPES.

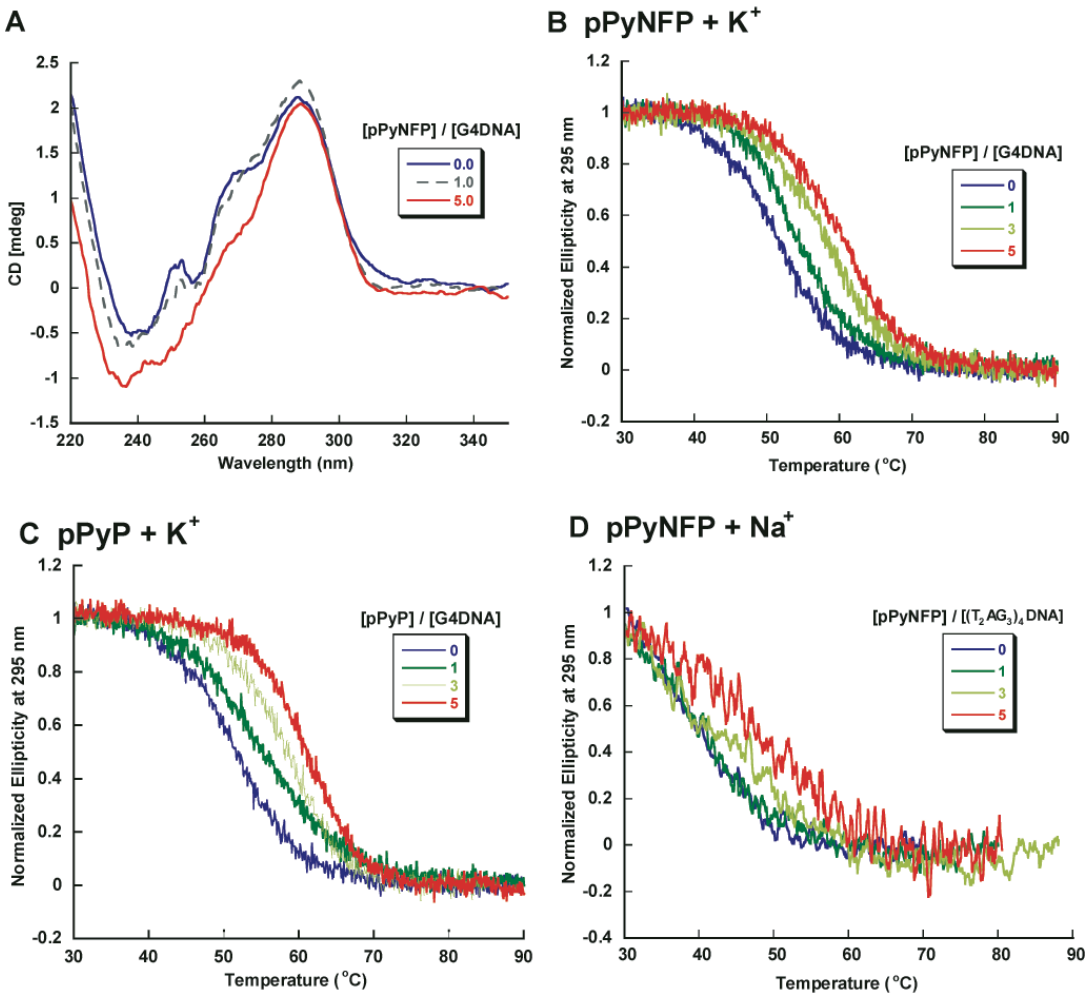


Fig. S5
CD analyses of G-quadruplex DNAs.

A: CD titration of G4 DNA forming a (3+1) parallel/antiparallel structure induced by 100 mM K^+ ions.
B: CD melting curves of 5.0 μM G4 DNA with different concentrations of **pPyNFP** (5.0, 15, and 25 μM) in 100 mM KCl at pH 7.4, 10 mM Tris-HCl, 1 mM EDTA buffer. CD spectra were monitored at 290 nm.
C: CD melting curves of 5.0 μM G4 DNA with different concentrations of **pPyP** (5.0, 15, and 25 μM) in 100 mM KCl at pH 7.4, 10 mM Tris-HCl, 1 mM EDTA buffer. CD spectra were monitored at 290 nm.
D: CD melting curves of 5.0 μM $(T_2AG_3)_4$ DNA with different concentrations of **pPyNFP** (5.0, 15, and 25 μM) in 100 mM NaCl at pH 7.4, 10 mM Tris-HCl, 1 mM EDTA buffer. CD spectra were monitored at 290 nm.

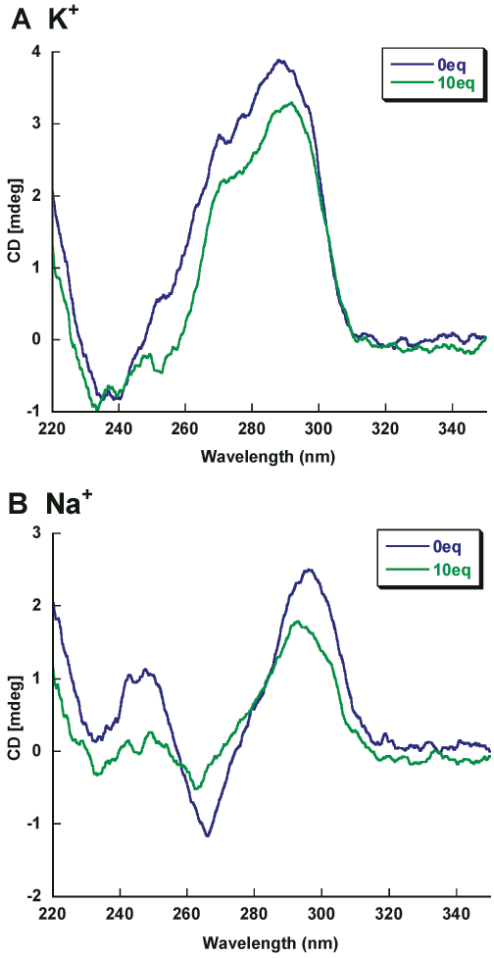


Fig. S6
Effects of **pPyP** on different G-quadruplex DNA structures.

A: CD titration of $(T_2AG_3)_4$ DNA forming a (3+1) parallel/antiparallel structure induced by 100 mM K^+ ions with 10 mM Tris-HCl (pH 7.4) and 1 mM EDTA.
B: CD titration of $(T_2AG_3)_4$ DNA forming a (2+2) antiparallel structure induced by 100 mM Na^+ ions with 10 mM Tris-HCl (pH 7.4) and 1 mM EDTA.

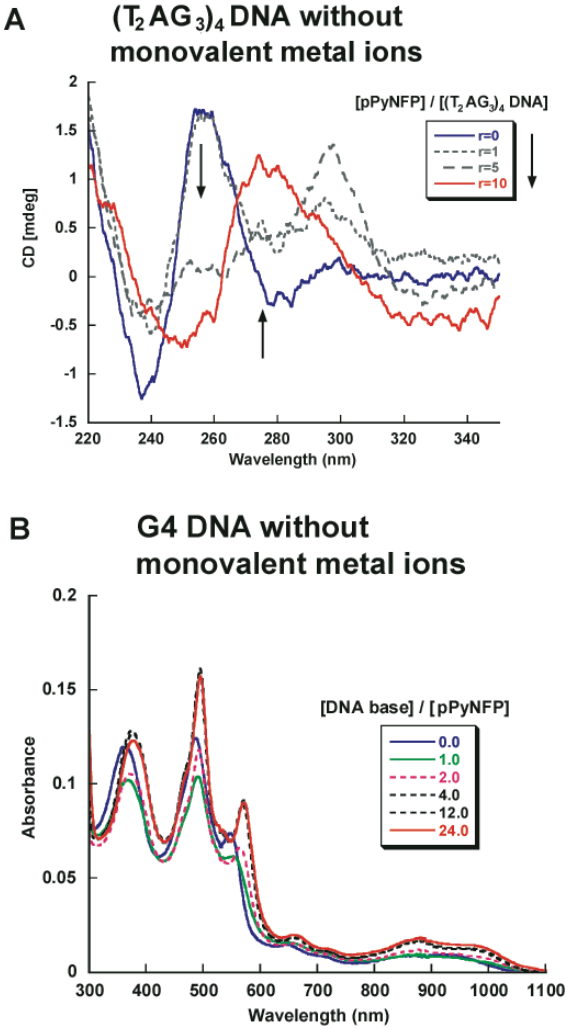


Fig. S7
Interaction between telomeric repeat DNA and **pPyNFP** in the absence of monovalent meal ions.

A: CD titration of $(T_2AG_3)_4$ DNA in the presence of 10 mM Tris-HCl (pH 7.4) and 1 mM EDTA.
B: UV-vis-NIR absorption of **pPyNFP** (7.5 μM) in the presence of different amounts of G4-DNA without monovalent metal ions (10 mM Tris-HCl (pH 7.4), 1 mM EDTA).

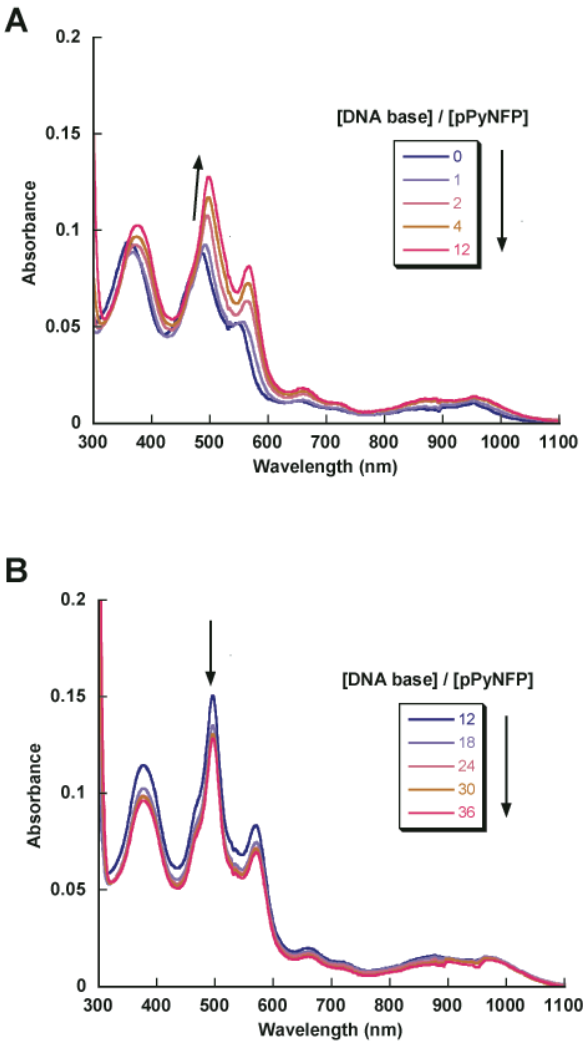
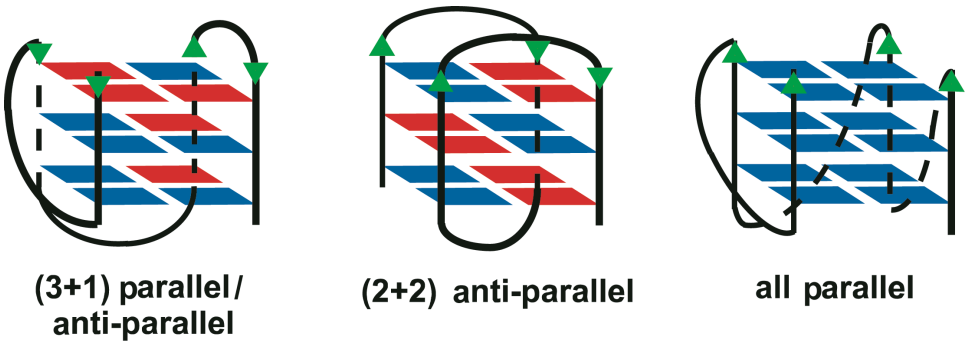


Fig. S8
Effects of the Na^+-induced (2+2) antiparallel structure on the absorption property of **pPyNFP**.

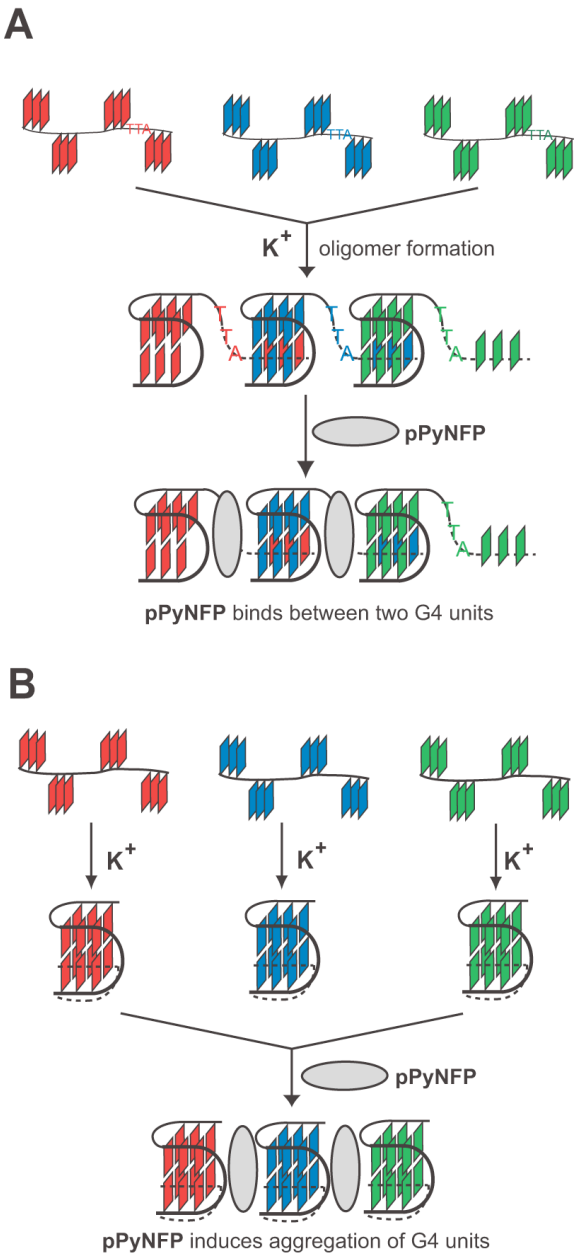
UV-vis-NIR absorption spectra of **pPyNFP** (7.5 μM) in the presence of less (A) or more (B) than 12 equivalent molar amount of DNA base (i.e. 0.5 equivalent molar amount of the (2+2) antiparallel DNA structure) induced by 100 mM Na^+ ions with 10 mM Tris-HCl (pH 7.4) and 1 mM EDTA.

Table S1
CD melting temperatures of $(T_2AG_3)_4$ DNA in the presence of 100 mM Na^+ and different concentration of **pPyNFP**

		r = [**pPyNFP**]/[$(T_2AG_3)_4$ DNA]			
		0 (DNA alone)	1	3	5
pPyNFP	T_m (°C)	40.0 ± 0.5	41.1 ± 0.2	42.7 ± 0.4	47.6 ± 0.3
	ΔT_m (°C)	–	1.1 ± 0.3	2.7 ± 0.2	7.6 ± 0.2



Scheme S1
Folding topologies of $(T_2AG_3)_4$ DNA. Glycosidic *anti* and *syn* conformations of guanines are colored blue and red, respectively.
A: K^+ ion dependent (3+1) parallel/antiparallel structure in solution.
B: Na^+ ion dependent (2+2) antiparallel structure induced in solution.
C: K^+ ion dependent all parallel structure induced in crystals.



Scheme S2

Possible models of interactions between **pPyNFP** and higher order G-quadruplexes.