Supporting Information for

1,10-Phenanthroline platinum(II) complex: simple molecule for efficient G-quadruplex stabilization

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Synthesis. All chemicals and solvent were obtained from commercial sources and used without further purification.

$[Pt(phen)_2](PF_6)_2$.[1] An aqueous suspension (40 mL) of $Pt(phen)Cl_2$[2] (45 mg, 0.1 mmol) and phenanthroline monohydrate ($phen \cdot H_2O$) (40 mg, 0.2 mmol) was stirred for 24 h at 108 °C until a clear yellow solution formed. Then $NaPF_6$ (35 mg, 0.21 mmol) was added to the solution and pale yellow $[Pt(phen)_2](PF_6)_2$ precipitated immediately. The product was filtered through a Teflon® filter (pore diameter 1 μm), washed two times with 20 mL water in the filter and dried under vacuum (36 mg, 42.8 % yield). Anal. calcd (%) for $C_{24}H_{16}F_{12}N_4P_2Pt$: C 34.10, H 1.91, N 6.63. Found: C 34.38, H 2.10, N 6.73. ^{1}H NMR (300 MHz, [*D*6]DMSO): δ = 9.493 (d, 2 H, *J* = 5.7 Hz), 9.014 (d, 2 H, *J* = 8.1 Hz), 8.313 (s, 2 H), 8.088 (dd, 2 H, J_1 = 8.1 Hz, J_2 = 2.4 Hz).

$[Pt(bpy)_2](PF_6)_2$.[1] This was prepared using the same procedure as for complex **1**, except that 0.15 mmol 2,2′-bipyridine. Yield 32.6 %. Anal. calcd (%) for $C_{20}H_{16}F_{12}N_4P_2Pt$: C 30.13, H 2.02, N 7.03. Found: C 30.09, H 2.18, N 6.98. ^{1}H NMR (300 MHz, [*D*6]DMSO): δ = 9.057 (d, 2 H, *J* = 5.4 Hz), 8.795 (d, 2 H, *J* = 7.8 Hz), 8.607 (t, 2 H, *J* = 7.8 Hz), 8.015 (t, 2 H, *J* = 6.3 Hz,).

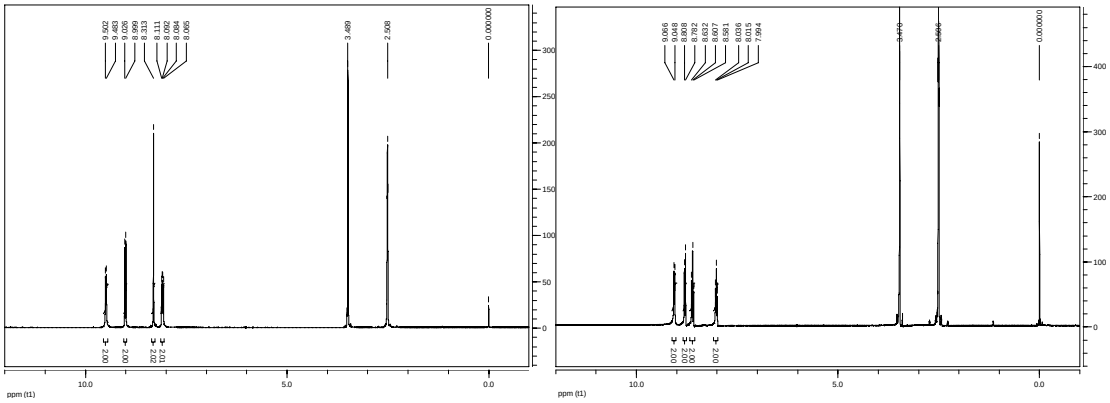

Fig. S1. ^{1}H NMR spectra of complexes **1** (left) and **2** (right).

CD spectroscopy. CD measurements were recorded on a Jasco J-810 CD spectropolarimeter at room temperature using a cell length of 1 cm, and over a wavelength range of 220-350 nm. The oligomer 22AG (5'-$AG_3(T_2AG_3)_3$-3') at a final concentration of 3 μM was resuspended in Tris-HCl buffer (10 mM, pH 7.4) containing 100 mM K^+ or not and the complexes to be tested. The samples were heated to 95 °C for 5 min, then gradually cooled to room temperature and incubated at 4 °C overnight. CD spectra were baseline-corrected for signal contributions due to the buffer. CD titration was performed at a fixed 22AG concentration (3 μM) with various concentrations of the complexes (3 mM in DMSO). After each addition of complex, the reaction was stirred and allowed to equilibrate for at least 10 min (until no elliptic changes were observed) and a CD spectrum was collected at least five scans. Final analysis of the data was carried out using Origin 7.5 (OriginLab Corp.).

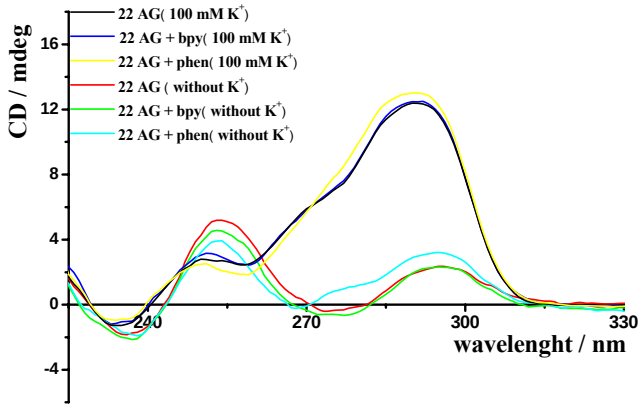

Fig. S2. CD spectra of 22AG quadruplex (3 μM) in the presence of bpy (3 μM) and phen (3 μM) in 10 mM Tris-HCl buffer, pH 7.4, 100 mM KCl and no metal cations, rt.

Fluorescence resonance energy transfer (FRET) studies. The fluorescent labeled oligonucleotide F21T (5′- *FAM*-$G_3[T_2AG_3]_3$-*TAMRA*-3′, FAM: 6-carboxyfluorescein, TAMRA: 6-carboxy-tetramethylrhodamine] used as the FRET probes were diluted in Tris-HCl buffer (10 mM, pH 7.4) containing 60 mM KCl and then annealed by heating to 92 °C for 5 min, followed by cooling slowly to room temperature overnight. Fluorescence melting curves were determined with a Bio-Rad iQ5 real-time PCR detection system, using a total reaction volume of 25 μL, with 0.4 μM of labeled oligonucleotide and different concentrations of complexes in Tris-HCl buffer (10 mM, pH 7.4)

containing 60 mM KCl. A constant temperature maintained for 30 s prior to each reading to ensure a stable value. Final analysis of the data was carried out using Origin 7.5 (OriginLab Corp.).

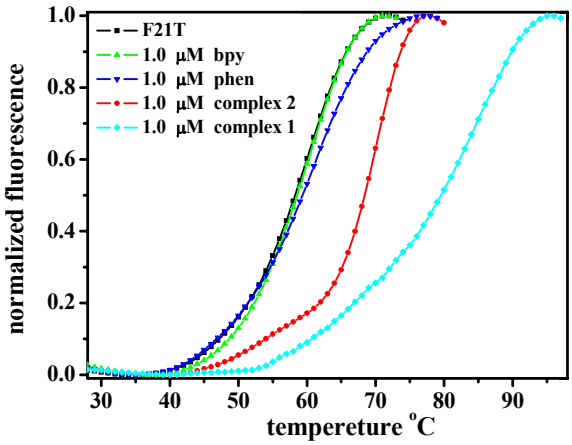

Fig. S3. FRET-melting curves obtained with F21T (0.4 μM) alone (■) and with 1μM of bpy(▲), phen(▼), $[Pt(bpy)_2](PF_6)_2$(●) and $[Pt(phen)_2](PF_6)_2$(□).

PCR stop assay. The oligonucleotide HTG21 (5'-$G_3(T_2AG_3)_3$-3') and the corresponding complementary sequence (HTG21rev, $ATCGCT_2CTCGTC_3TA_2C_2$) were used here. The reactions were performed in 1× PCR buffer, containing 10 pmol of each oligonucleotide, 0.16 mM dNTP, 2.5 U *Taq* polymerase, and different concentrations of complexes. Reaction mixtures were incubated in a thermocycler with the following cycling conditions: 94 °C for 3 min, followed by 30 cycles of 94 °C for 30 s, 58 °C for 30 s, and 72 °C for 30 s. PCR products were then analysed on 15% nondenaturing polyacrylamide gels in 1× TBE and silver stained.

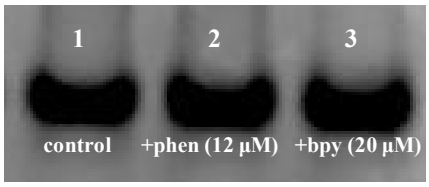

Fig. S4. Effect of the two ligands on the hybridization of HTG 21 in the PCR-stop assay.

1 C. Finazzo, M. Fontana, S. Van Doorslaer, W. Caseri and A. Schweiger, *Phys. Chem. Chem. Phys.*, 2005, **7**, 405.

2 G.T. Morgan and F.H. Burstall, *J. Chem. Soc.*, 1934, 965.