Supplementary Information

Metal Ions Modulate the Conformation and Stability of G-Quadruplex with or without a Small-Molecule Ligand

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Supplementary methods

Absorption spectra study with compound 4

The absorption titration of compound **4** was performed by using a fixed concentration (1 μM) of the ligand in buffer (10 mM Tris-HCl + 100 mM KCl, pH 7.4) and increasing concentrations of the G-quadruplex. The solutions were mixed and incubated for 2 h at room temperature before absorption spectra were recorded. UV absorption spectra were obtained by using a Shimadzu UV-3600 spectrophotometer. UV absorption spectra showed that after adding G-quadruplex, a hypochromic effect as well as a redshift of approximately 7 nm of the characteristic absorption band of compound **4** occurred (Fig. S5), indicating the intercalation of the compound into G-quadruplex. The binding constant of compound **4** with G-quadruplex was 4.84×10^{8} M^{-1}. The binding constant has been calculated from the equation.[1]

$$C_{G4}/(\varepsilon_a - \varepsilon_f) = C_{G4}/(\varepsilon_b - \varepsilon_f) + 1/(K(\varepsilon_b - \varepsilon_f))$$

Where ε_a corresponds to $A_{obsd}/C_{compound\ 4}$, ε_f corresponds to extinction coefficient for the free compound **4**, ε_b corresponds the extinction coefficient for the compound **4** complex in the fully bound form.

References

1. A. M. Pyle, J. P. Rehmann, R. Meshoyrer, C. V. Kumar, N. J. Turro and J. K. Barton, *J. Am. Chem. Soc.*, 1989, **111**, 3051-3058.

Supplementary Figures

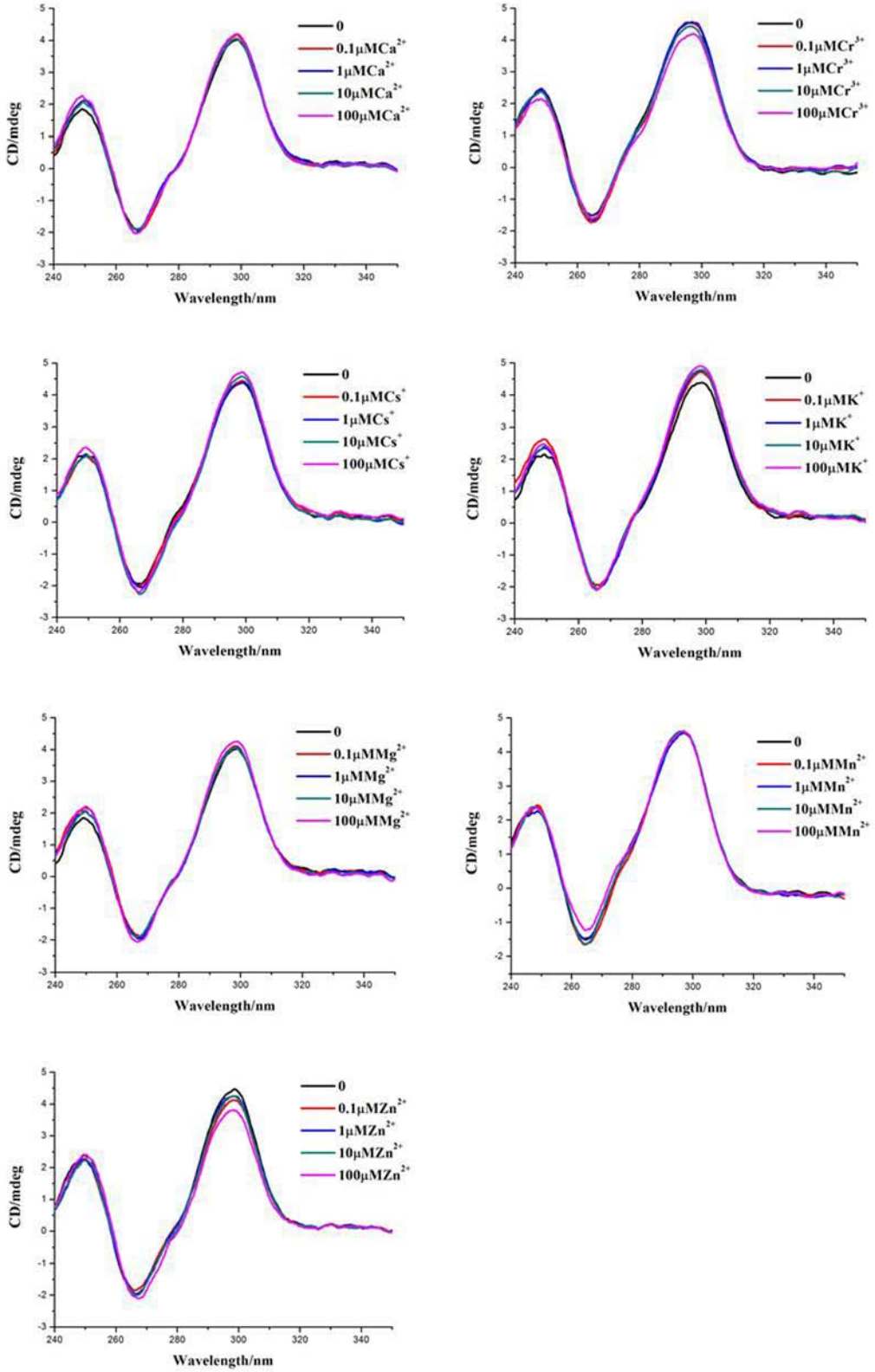

Fig. S1 CD spectra of Na^{+}-induced G-quadruplex (1 μM) with increasing concentrations of Ca^{2+}, Cr^{3+}, Cs^{+}, K^{+}, Mg^{2+}, Mn^{2+}, or Zn^{2+} in 50 mM NaAc and 10mM Tris-HAc buffer, pH 7.4.

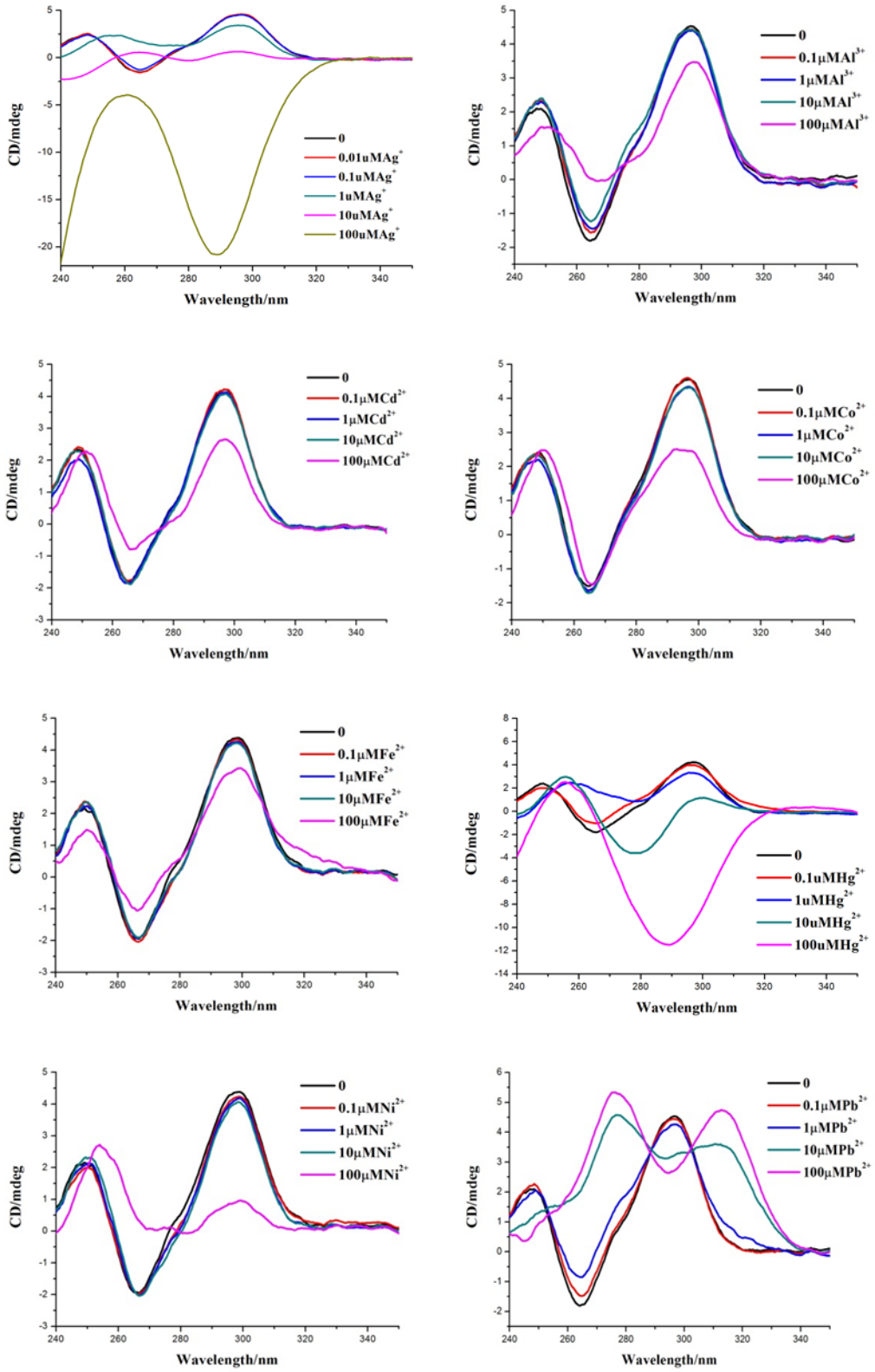

Fig. S2 CD spectra of Na^{+}-induced G-quadruplex (1 μM) with increasing concentrations of Ag^{+}, Al^{3+}, Cd^{2+}, Co^{2+}, Fe^{2+}, Hg^{2+}, Ni^{2+}, or Pb^{2+} in 50 mM NaAc and 10mM Tris-HAc buffer, pH 7.4.

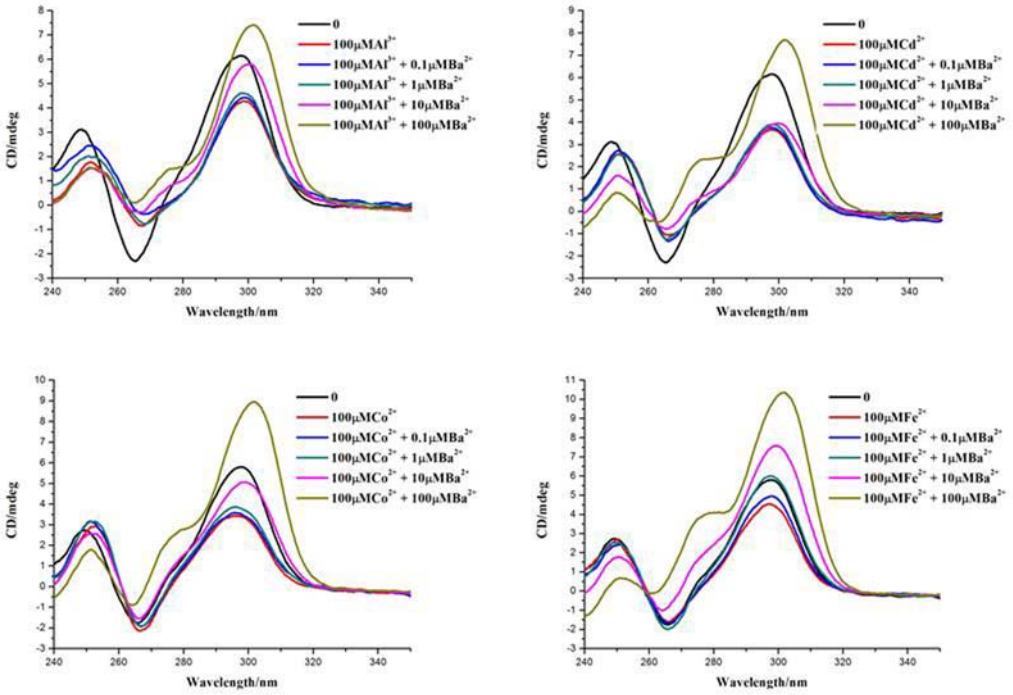

Fig. S3 CD spectra of Na^{+}-induced G-quadruplex (1 μM) with 100 μM of Al^{3+}、Cd^{2+}、Co^{2+}、or Fe^{2+} and increasing concentrations of Ba^{2+} in 50 mM NaAc and 10 mM Tris-HAc buffer, pH 7.4.

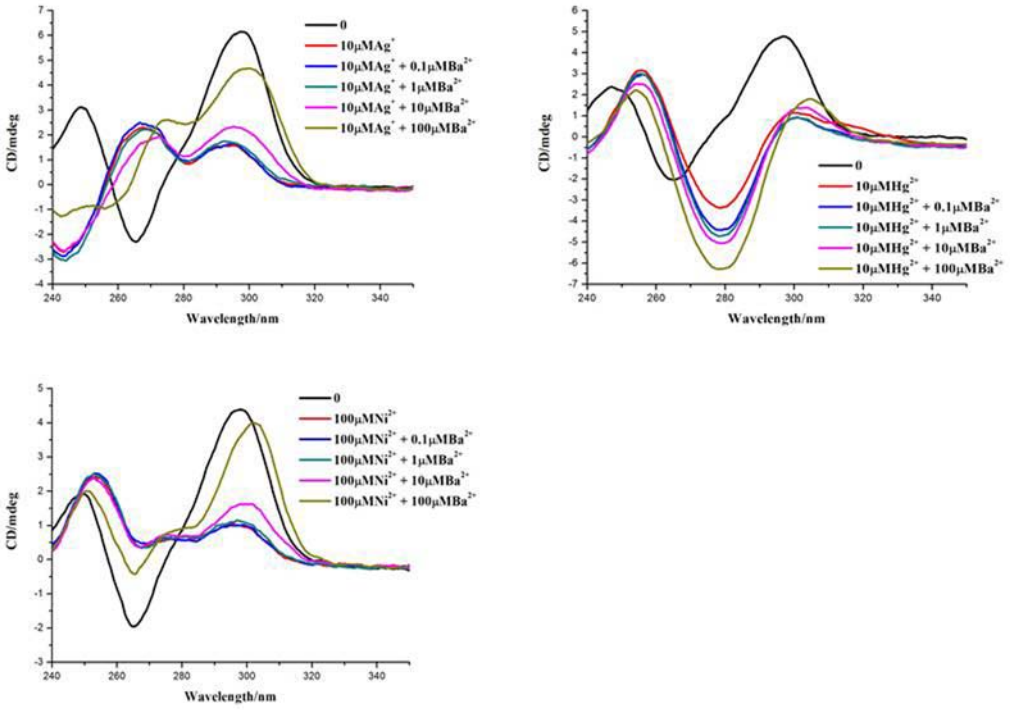

Fig. S4 CD spectra of Na^{+}-induced G-quadruplex (1 μM) with Ag^{+}, Hg^{2+}, or Ni^{2+} and increasing concentrations of Ba^{2+} in 50 mM NaAc and 10 mM Tris-HAc buffer, pH 7.4.

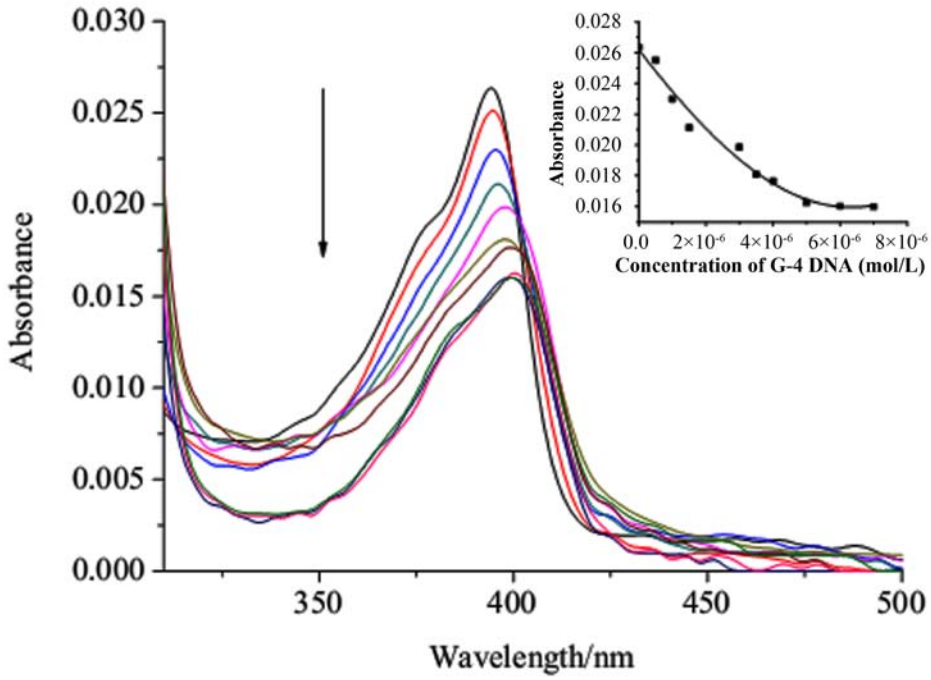

Fig. S5 UV absorption spectra of compound **4** (1 μM) with increasing concentrations of G-quadruplex.

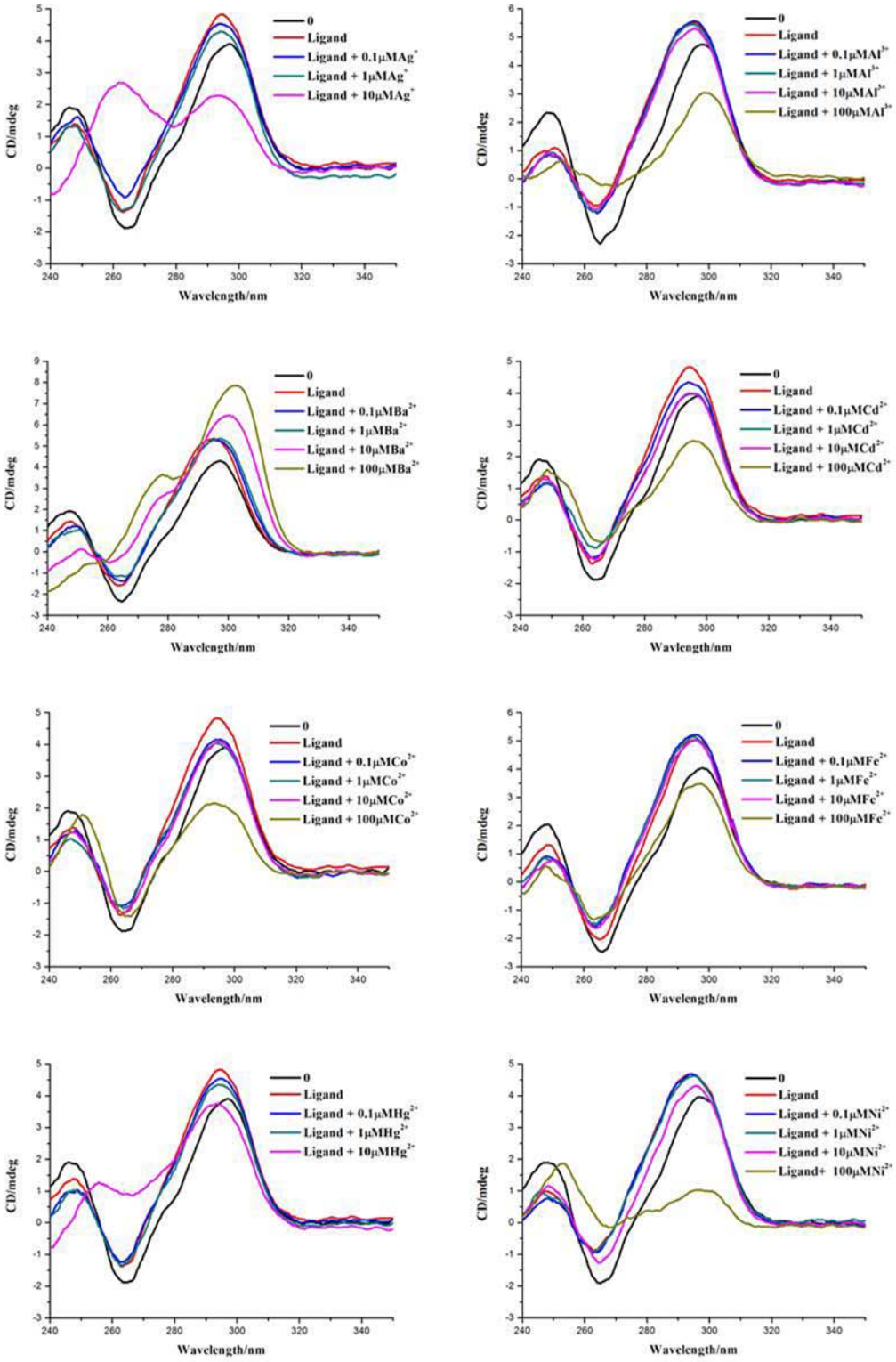

Fig. S6 CD spectra of Na^{+}-induced G-quadruplex with compound **4** (3 μM) and increasing concentrations of Ag^{+}, Al^{3+}, Ba^{2+}, Cd^{2+}, Co^{2+}, Fe^{2+}, Hg^{2+}, or Ni^{2+} in 50 mM NaAc and 10 mM Tris-HAc buffer, pH 7.4.

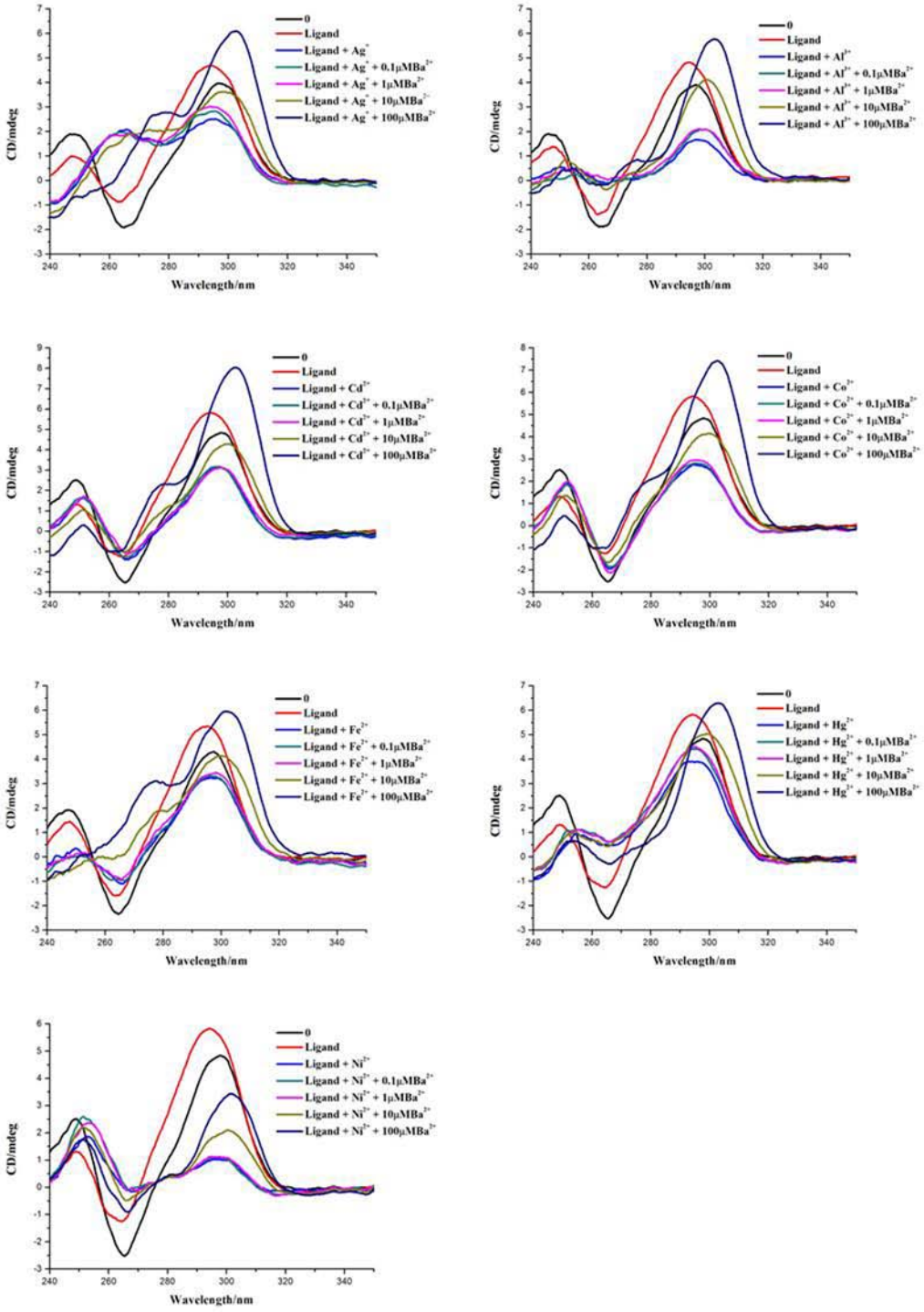

Fig. S7 CD spectra of Na^{+}-induced G-quadruplex in the presence of compound **4** (3 μM) and 100 μM of Al^{3+}, Cd^{2+}, Co^{2+}, Fe^{2+}, Ni^{2+}, or 10 μM of Ag^{+} or Hg^{2+}, and increasing concentrations of Ba^{2+} in 50 mM NaAc and 10 mM Tris-HAc buffer, pH 7.4.

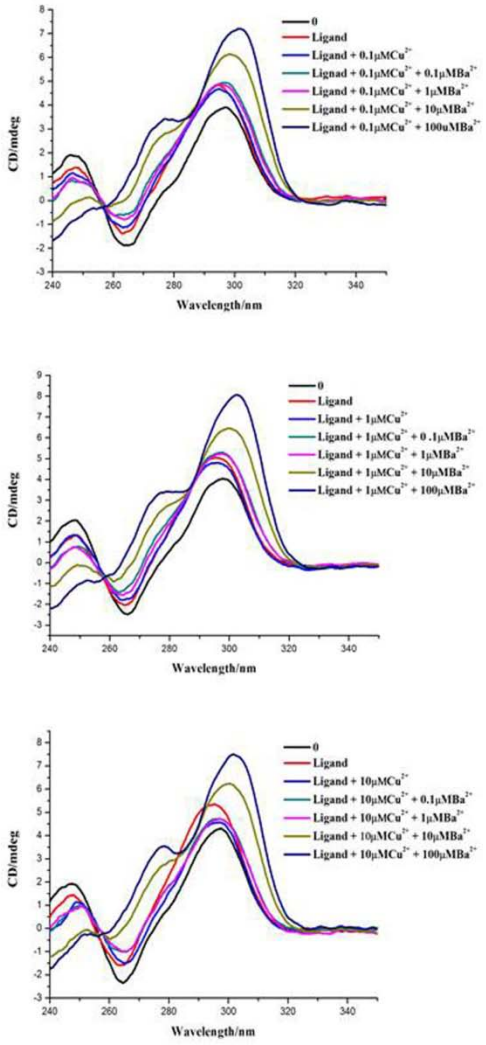

Fig. S8 CD spectra of Na^{+}-induced G-quadruplex in the presence of compound **4** (3 μM) and 0.1, 1 or 10 μM of Cu^{2+}, with increasing concentrations of Ba^{2+} in 50 mM NaAc and 10 mM Tris-HAc buffer, pH 7.4.

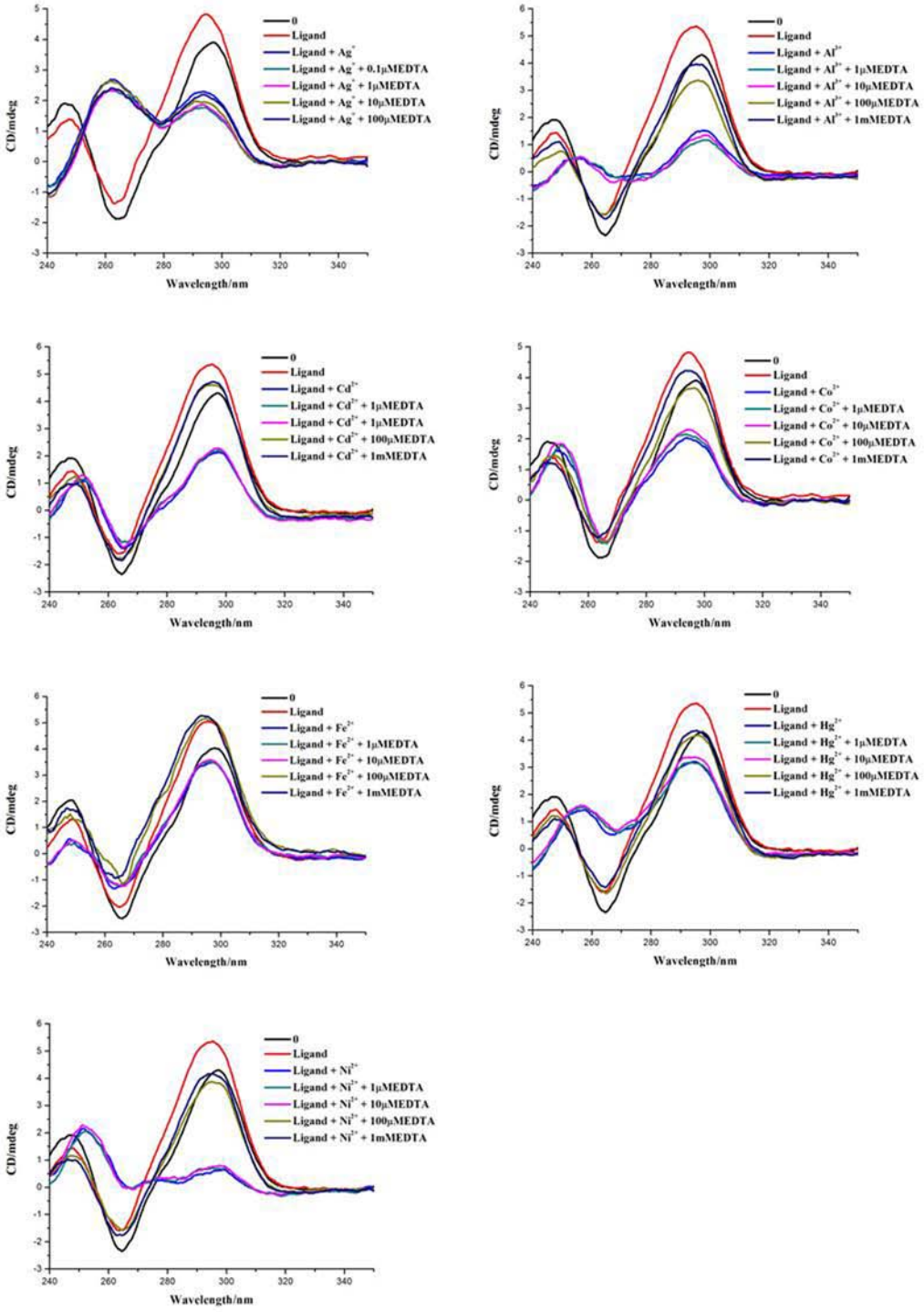

Fig. S9 CD spectra of Na^+-induced G-quadruplex in the presence of compound **4** (3 μM) and 100 μM of Al^{3+}, Cd^{2+}, Co^{2+}, Fe^{2+}, Ni^{2+}, or 10 μM of Ag^+ or Hg^{2+}, with increasing concentrations of EDTA in 50 mM NaAc and 10 mM Tris-HAc buffer, pH 7.4.