Electronic Supplementary Material (ESI) for ChemComm.

Electronic supplementary information

Probing metal-dependent G-quadruplexes using the intrinsic fluorescence of DNA

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Materials and Methods

All DNA sequences were purchased from Integrated DNA Technologies (Coralville, Iowa), dissolved in Milli-Q water at a stock concentration of 100 μM, and used without further purification. Potassium chloride (KCl), sodium chloride (NaCl) and calcium chloride ($CaCl_2$) were purchased from VWR Canada. Lead (Pb^{2+}) acetate, strontium chloride hexahydrate ($SrCl_2.6H_2O$), barium chloride dihydrate ($BaCl_2.2H_2O$), caesium chloride (CsCl), lithium chloride (LiCl) and thioflavin T(ThT) were purchased from Sigma-Aldrich. KCl was prepared to a stock concentration of 3M, while lead acetate was prepared to a stock concentration of 100 μM. All other ions were prepared to a stock concentration of 100 mM. Prior to measurement, each DNA was diluted to a working concentration of 5 μM.

Measurement of Fluorescence Spectra.

In a typical experiment, 200 μL of working DNA solution was placed in a 1 cm × 0.2 cm cuvette and the fluorescence was measured using a HORIBA Jobin–Yvon FluoroMax-3 spectrofluorimeter. Slit widths for both excitation and emission monochromators were set at 5 nm. Data integration was set at 0.2 s with a 1 nm data pitch for steady-state spectra. For kinetics experiments, fluorescence was measured every 30 seconds for 30 minutes, with excitation and emission set for the specific sequence. The fluorescence was measured for 5 min (to ensure stability) before the addition of K^+, Pb^{2+}, or any other metal ions. The fluorescence was then followed for the remaining 25 min. Excitation wavelengths were DNA-dependent, with PS2.M, PW17 and T30695 being excited at 290 nm, K^+ aptamer at 295 nm and A_{30} at 300 nm. ThT measurements were similar to above, except 5 μM ThT was added prior to the measurement, and the excitation was set at 425 nm (detecting at 490 nm for kinetics experiments), with slit widths at 1 nm.

A_{30} Purification

A Sep Pak C_{18} column was hydrated using solvents of increasing polarity, followed by the addition of 200 μL of a 20 μM A_{30} solution. The eluate was collected and re-added to the column 7 times, and the final eluate was discarded. Then, the column was rinsed with 2 × 10 mL aliquots of Milli-Q water. Finally, the bound DNA was eluted using 1 mL of 1:1:1 acetonitile:methanol:H_2O solution and a 95% acetonitrile solution. The eluate was lyophilized under vacuum centrifugation and resuspended in Milli-Q water. The fluorescence before and after purification was measured by a Cary Eclipse (Varian) fluorimeter. The UV/Vis spectra was collected by an Agilent 8453A spectrophotometer.

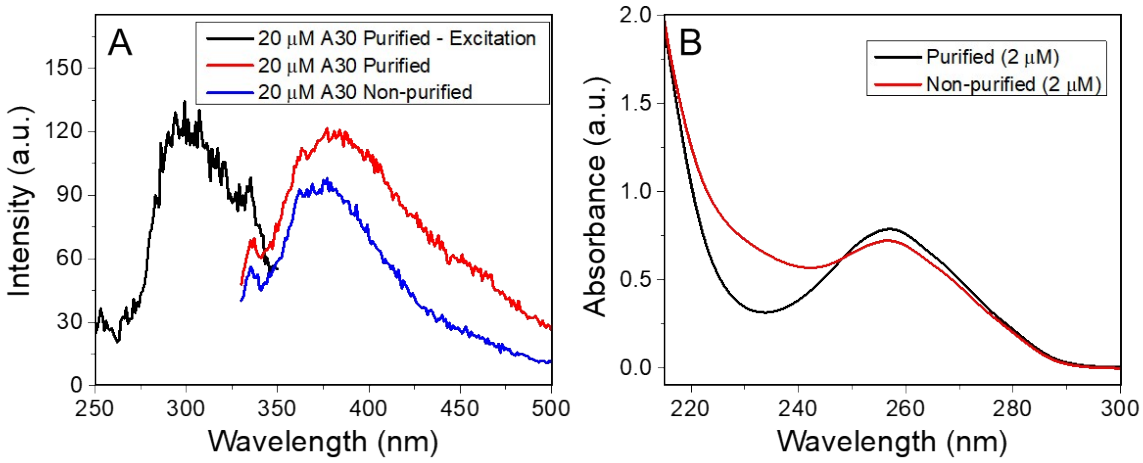

Figure S1. (A) Fluorescence and (B) UV/Vis spectra of A_{30} DNA before and after purification with reverse-phase chromatography. Excitation at 300 nm was used for emission spectra.

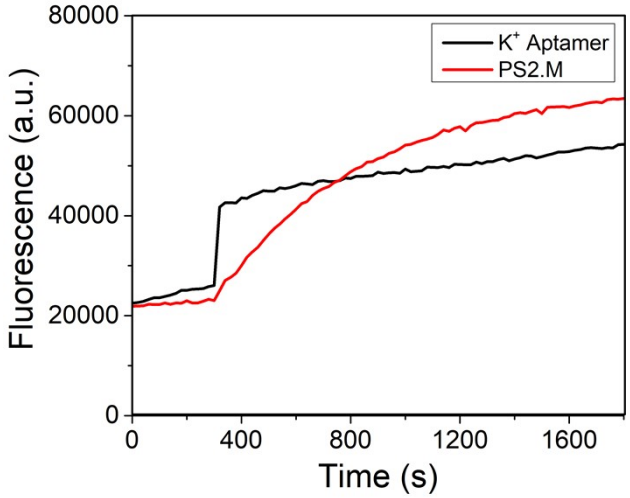

Figure S2. Response of the intrinsic fluorescence of 5 μM K^+ aptamer and PS2.M to 60 mM K^+.

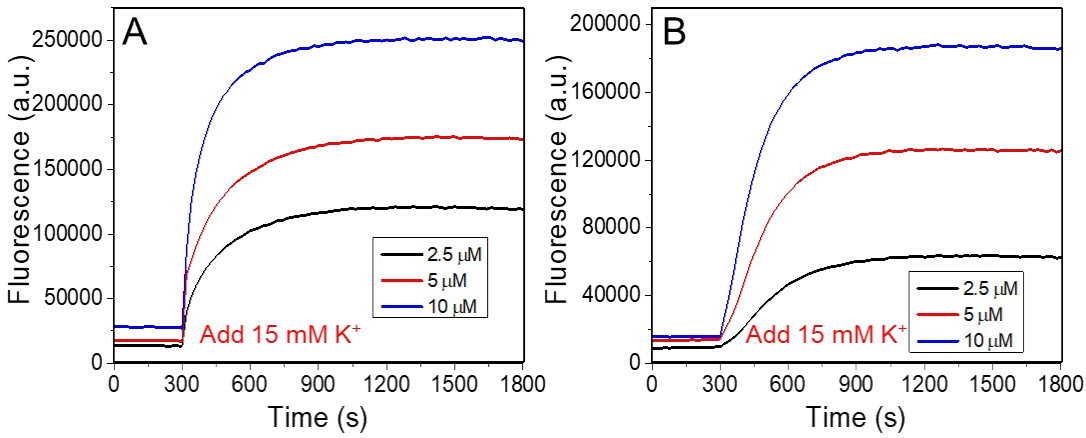

Figure S3. Kinetics of fluorescence change of (A) T30695 and (B) PW17 as a function of DNA concentration upon the addition of 15 mM K^+ at 300 sec in Milli-Q water.

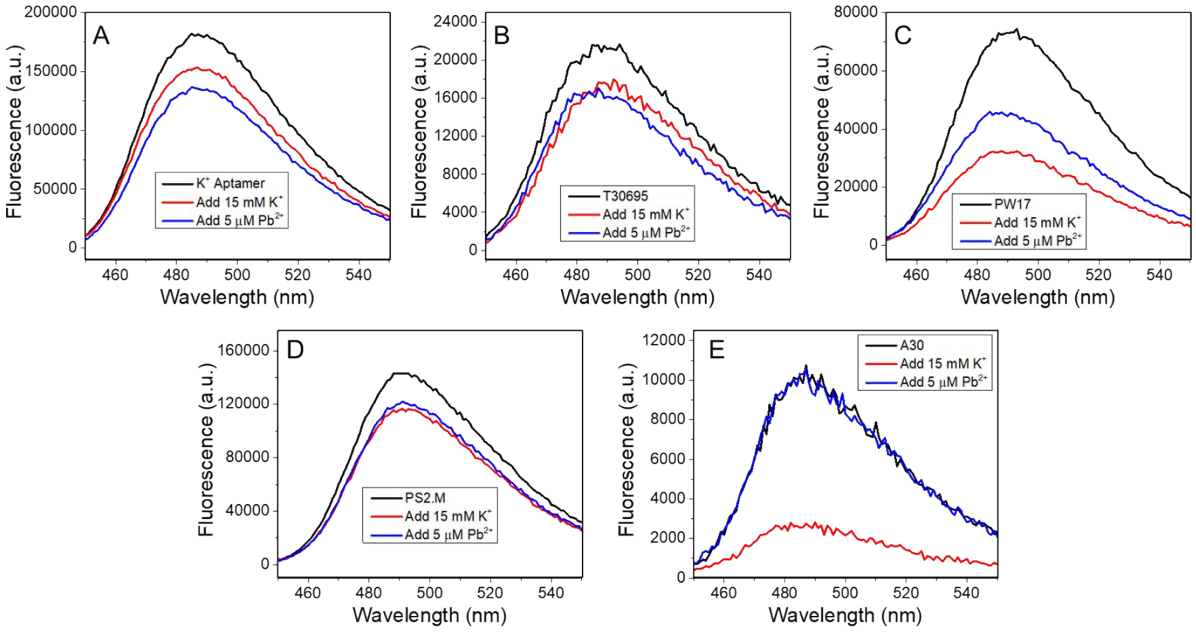

Figure S4. ThT fluorescence spectra with (A) K^+ aptamer, (B) T30695, (C) PW17, (D) PS2.M, and (E) A_{30} in Milli-Q water. Excitation was at 425 nm.

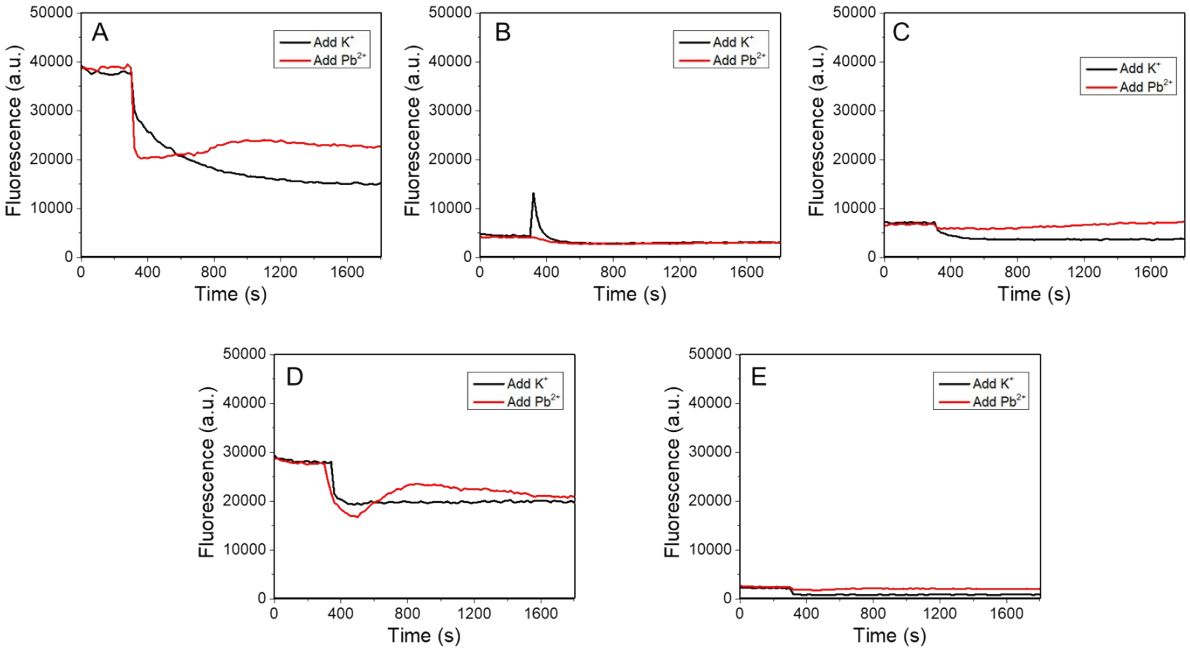

Figure S5. ThT fluorescence kinetics for (A) K^+ aptamer, (B) T30695, (C) PW17, (D) PS2.M, (E) A_{30} in Milli-Q water. Excitation was at 425 nm and emission was set at 490 nm.

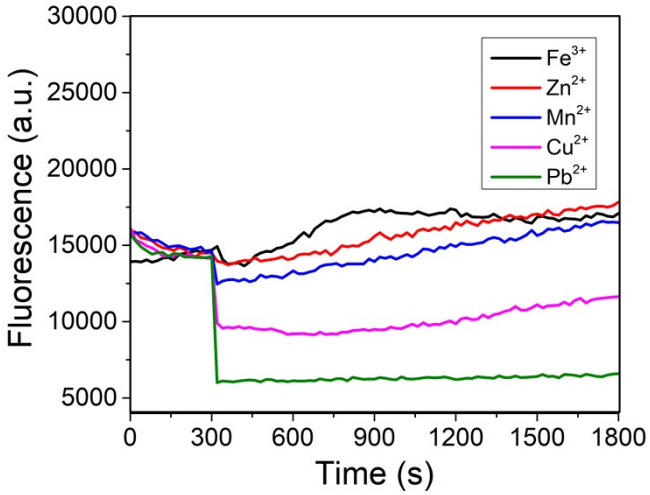

Figure S6. Response of 5 μM T30695 to 5 μM of different metal ions.