# A colorimetric and fluorometric dual-modal DNA logic gate based on the recognition of a cyanine dye supramolecule to G-quadruplexes

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## Materials and Methods

**Sample Preparation.** The cyanine dye MTC was synthesized according to Hamer's[1] and Brooker's[2] methods, and the purity was evaluated by mass spectrometry and nuclear magnetic resonance. The G-rich oligonucleotides, PS2.M (GTGGGTAGGGCGGGTTGG), were obtained from Sangon Biotechnology Co., Ltd. (Shanghai, China) and purified by HPLC. The metal salt (KCl), methanol, and Tris (Tris(hydroxymethyl)aminomethane) were all analytical grade, being purchased from Beijing Chemical Company and used without further purification. $Pb^{2+}$ standard solution (1000 μg/mL) was purchased from General Research Institute for Nonferrous Metals of China.

Ultrapure water used throughout the experiments was prepared by Milli-Q Gradient ultrapure water system (Millipore; 18.2 MΩ). The stock solution of MTC was prepared by dissolving it in methanol to 200 μM and then stored in the dark. The stock solutions of the oligonucleotides were prepared by dissolving oligonucleotides directly into 10 mM Tris-HCl buffer solution (pH 7.2). The DNA sample had been stored for more than 24 h at 4℃ and then structurally identified by the circular dichroism (CD) spectra. The concentrations of DNA stock solutions were determined by measuring their absorbance at 260 nm before using.

The solution is prepared with next several steps. Firstly, adding the 10 mM Tris-HCl buffer solution containing into the MTC solution to prepare MTC aggregates (the volume of the Tris-HCl buffer solution is 10-fold of the MTC mother solution). Secondly, titrate PS2.M solution into MTC solution. Then, add different inputs into the system. These mixtures were prepared at room temperature.

**Spectroscopy Measurement.** Ultraviolet (UV) spectra was measured on an Agilent 8453 UV-visible spectrophotometer at the wavelength range 190-1100 nm using a 1 cm path cell at room temperature (25°C). Ultrapure water was used as reference.

Fluorescence spectra experiments were conducted on a Hitachi F-4500 spectrofluorometer (Japan) in a 10 mm path-length quartz cell at room temperature.

Xenon arc lamp was used as the excitation light source. Both excitation and emission slits were 10 nm and the scan speed was 1200 nm/min. Excitation was set at 570 nm, and emission was collected from 580 nm to 700 nm.

CD spectra were collected from 200 to 350 nm on a Jasco-815 automatic recording spectropolarimeter with a 1cm path-length quartz cell at 25 ºC. Spectra was collected with scan speed of 1000nm/min. Each spectrum was the average of three scans. A solution containing no oligonucleotide was used as reference, and a buffer blank correction was made for all spectra. The cuvette-holding chamber was flushed with a constant stream of dry $N_2$ gas to avoid water condensation on the cuvette exterior.

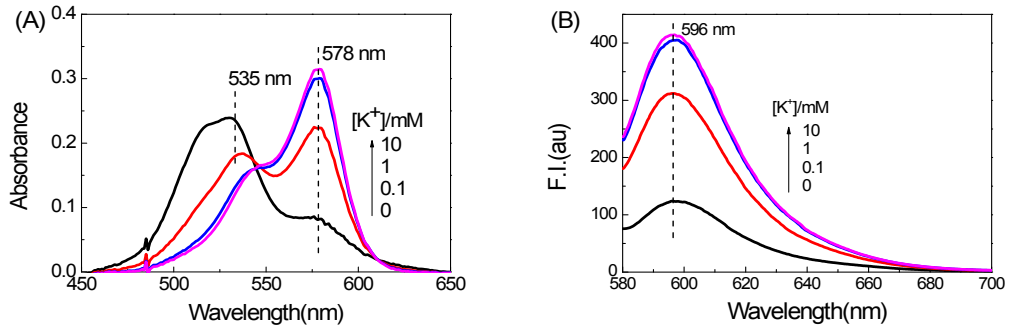


**Figure S1.** (A) The absorption spectra and (B) the fluorescence spectra of 4 μM MTC with increasing concentrations of $K^+$ in 10 mM Tris-HCl containing 2 μM PS2.M.

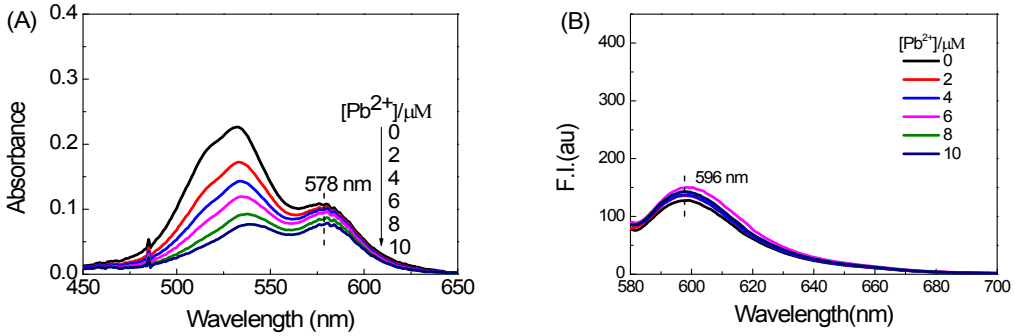


**Figure S2.** (A) The absorption spectra and (B) the fluorescence spectra of 4 μM MTC with increasing $Pb^{2+}$ in 10 mM Tris-HCl containing 2 μM PS2.M.

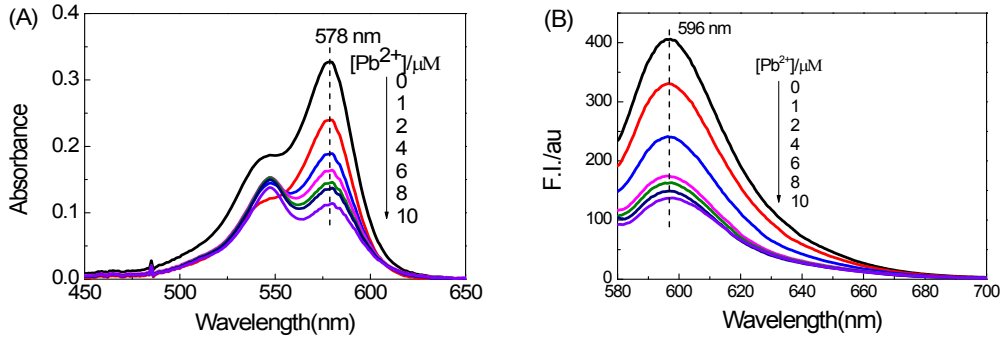


**Figure S3.** (A) The absorption spectra and (B) the fluorescence spectra of 4 μM MTC with increasing $Pb^{2+}$ in 10 mM Tris-HCl containing 2 μM PS2.M and 10 mM $K^{+}$.

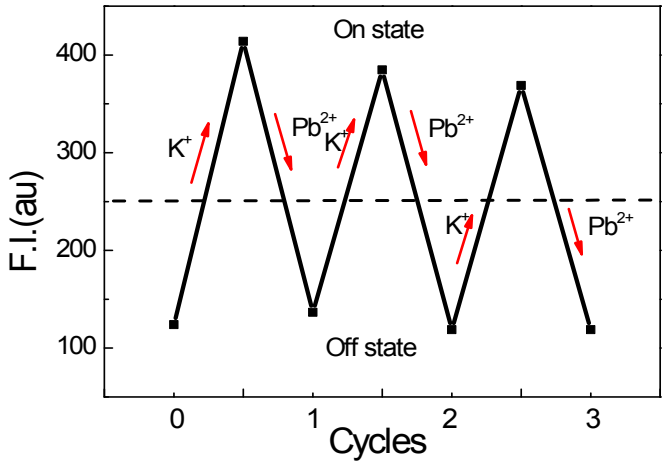


**Figure S4.** Reversible switching of the logic gate between the on and off states through the addition of $K^{+}$ and $Pb^{2+}$ in 10 mM Tris-HCl containing 2 μM PS2.M and 4 μM MTC.

## Notes and references

1. Hamer F M. The Chemistry of Heterocyclic Compounds . New York: Interscience, **1964**: 148-200.
2. Ficken G E. The Chemistry of Synthetic Dyes. New York: Academic Press, **1971**: 228-240**.**