Electronic Supplementary Information (ESI)

Berberine as a novel light-up i-motif fluorescence ligand and its application to design molecular logic systems

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Reagents

DNA oligomers were obtained from Sangon Biotechnology Co., Ltd. (Shanghai, China). hTeloC: 5'- TAACCCTAACCCTAACCCTAACCC -3'.

The DNA samples were prepared in ultrapure water, and the concentrations of DNA samples were accurately quantified using 260 nm UV absorbance. Berberine chloride was purchased from Aladdin Industrial Inc. (Shanghai, China). Other chemical reagents were of analytical grade and purchased from Sinopharm Chemical Reagent Co. Ltd. (Shanghai, China). 10 mM PB buffer (Na_2HPO_4/KH_2PO_4) was used in the experiment, if not particularly indicated. Milli-Q water was used to prepare solutions.

Instruments and Methods

F-4600 fluorescence spectrometer (Hitachi, Tokyo, Japan) was employed to record fluorescence spectra. The excitation wavelength was fixed at 350 nm and fluorescence emission spectra were collected from 450 to 670 nm for berberine. UV/Vis absorption spectra were recorded on a Lambda 25 spectrometer (PerkinElmer, Singapore) from 320 to 500 nm. The CD spectra were collected by a Chirascan-plus Circular Dichroism Spectrometer (Applied Photophysics Ltd, Surrey, UK). Three scans from 220 to 320 at 0.1 nm intervals were accumulated and averaged.

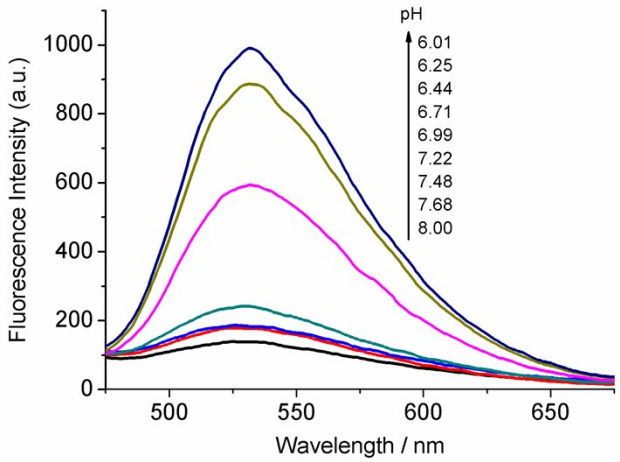

Figure S1. Fluorescence spectra of the berberine/hTeloC system in 10 mM PB buffer with different pH (6.01-8.00). [hTeloC] = 2 μM, [berberine] = 2 μM.

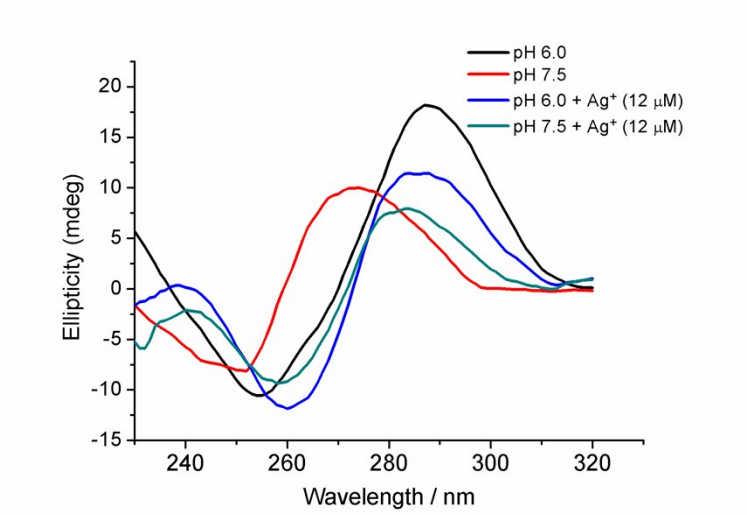

Figure S2. Circular dichroism (CD) spectrum of hTeloC (2 μM) in different conditions. Solutions were prepared in 10 mM PB buffer.

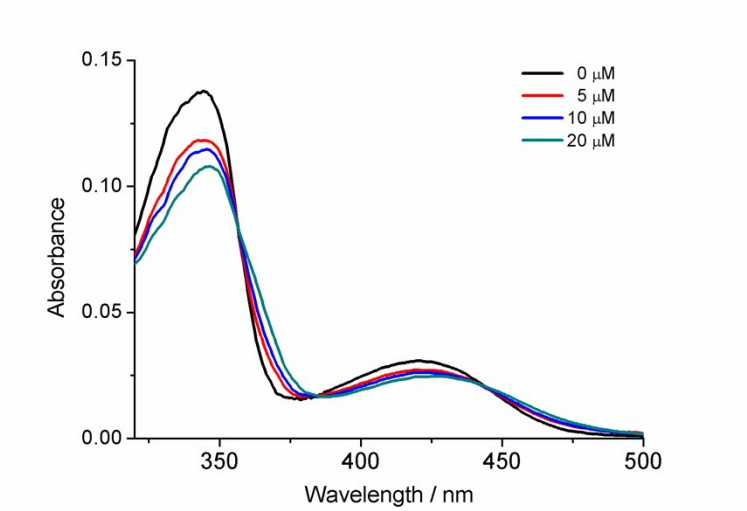

Figure S3. Absorption spectra of berberine (ca. 6 μM) with hTeloC (0, 5, 10, and 20 μM, respectively) in 10 mM PB buffer (pH 6.01).

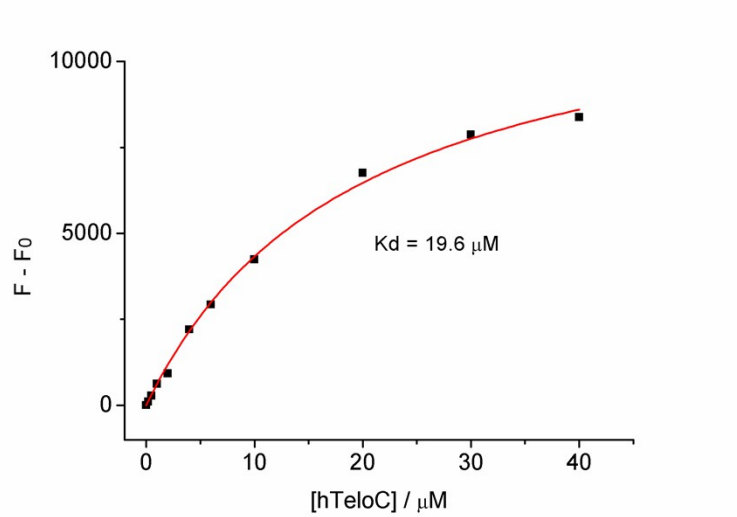

Figure S4. Nonlinear regression analysis of fluorescence binding curve of berberine (2 μM) with hTeloC in PB buffer (10 mM, pH 6.01) solution. F_0, F denotes the fluorescence intensity of berberine in the absence and presence of hTeloC, respectively. The excitation and maximum emission wavelengths were 350 nm and 530 nm, respectively.

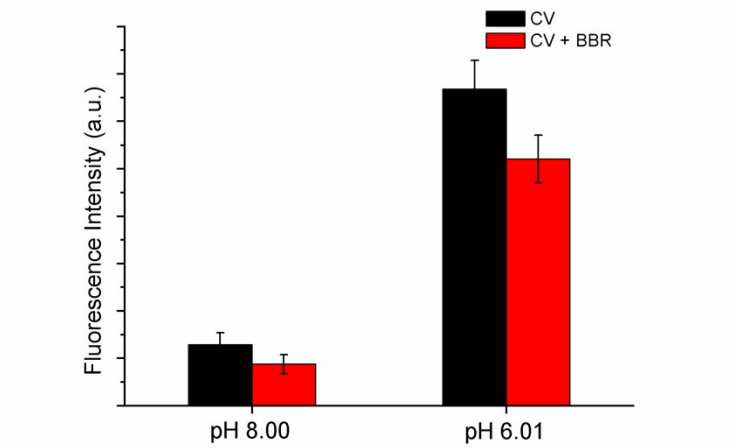

Figure S5. Fluorescence intensity at 625 nm of CV/C29 system in the absence and presence of BBR. The excitation wavelength was fixed at 580 nm. [CV] = [BBR] = [C29] = 2 μM. C29 has the following sequence: 5'- CCCCCTTTCCCCCTT TCCCCCTTTCCCCC -3'.

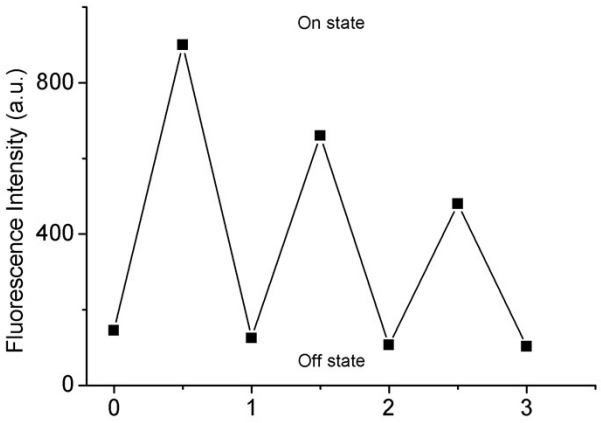

Figure S6. The reversible fluorescence response of the BBR/hTeloC system to pH. The solution pH was cycled between 6 and 8 by alternated addition of 0.2 M HNO_3 and 0.2 M NaOH.

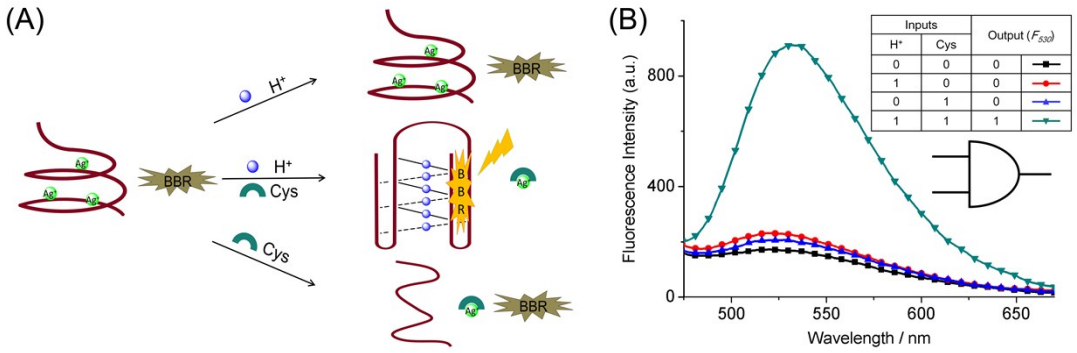

Figure S7. (A) Graphic illustration of the AND logic gate based on the BBR/hTeloC system in 10 mM PB buffer solution containing 15 μM Ag^+. (B) Fluorescence spectra of the AND logic gate with different inputs: ■, no input (pH 8.00); ●, H^+ (pH 6.01); ①, Cys (15 μM); or ②, H^+ (pH 6.01) + Cys (15 μM), and the corresponding truth table for the AND logic gate. [BBR] = [hTeloC] = 2 μM.

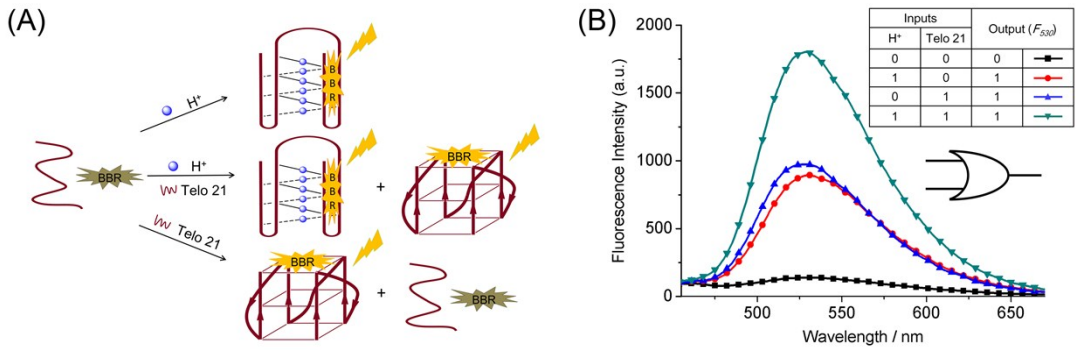

Figure S8. (A) Graphic illustration of the OR logic gate based on the BBR/hTeloC system in 10 mM PB buffer solution (Na_2HPO_4/NaH_2PO_4). (B) Fluorescence spectra of the OR logic gate with different inputs: ■, no input (pH 8.00); ●, H^+ (pH 6.01); ①, Telo 21 (0.3 μM); or ②, H^+ (pH 6.01) + Telo 21 (0.3 μM), and the corresponding truth table for the OR logic gate. [BBR] = [hTeloC] = 2 μM, [K^+] = 2 mM. Telo 21 has the following sequence: 5'-GGGTTAGGGTTAGGGTTAGGG -3'.

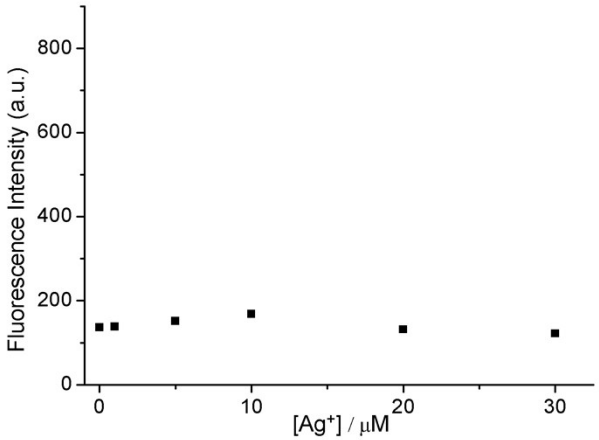

Figure S9. Fluorescence intensity at 530 nm of the BBR/hTeloC sensing system in the presence of different concentrations of Ag^+ in pH 8.00 PB buffer. [Berberine] = 2 μM, [hTeloC] = 2 μM, [Ag^+] = 0, 1, 5, 10, 20, and 30 μM, respectively.

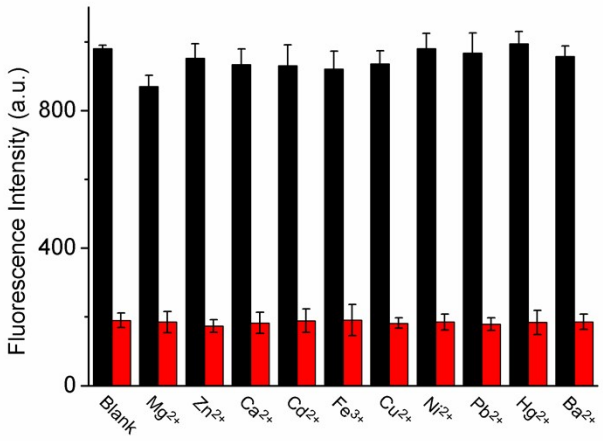

Figure S10. Specificity of the Ag^+ sensor. Black bars represent the fluorescence responses of this sensing system at 530 nm after addition of 15 μM of other metal ions. Red bars represent fluorescence responses of this sensing system at 530 nm after addition of 15 μM of Ag^+ together with 15 μM of one other metal ion. Solution: 10 mM PB buffer (pH 6.01) containing 1 mM EDTA as a masking agent. Error bars represent standard deviations from three repeated experiments.

Table S1 Detection of Ag^+ in tap water

Sample	Ag^+ added (μM)	Ag^+ found (μM)	Recovery(%)
1	20.0	19.77	98.9
2	30.0	34.52	115.1
3	40.0	44.90	112.3