Supporting Information

Materials

The synthetic oligonucleotide (listed in Table S1), adenosine triphosphate (ATP), cytidine triphosphate (CTP), guanosine triphosphate (GTP), and uridine triphosphate (UTP) were obtained from Sangon Biotechnology Co., Ltd (Shanghai, China). PPIX was purchased from Sigma-Aldrich. Other chemicals were of reagent grade and were used as received. The oligonucleotide was dissolved in water as stock solution and quantified by UV−Vis absorption spectroscopy with the following extinction coefficients (ε260 nm, $M^{-1}cm^{-1}$): A = 15400, G = 11500, C = 7400, T = 8700. UV-vis absorbance measurements were performed on a Cary 500 Scan UV/Vis/NIR Spectrophotometer (Varian, USA).

DNA Strand Displacement Reaction

TEK buffer (5 mM Tris-HCl, 0.5 mM EDTA, 100 mM NaCl, 20 mM KCl, 10 mM $MgCl_2$, pH 8.0) was used in this system for hybridization of strands and formation of G-quadruplex. In strand displacement reaction, the solutions of strand S and M were mixed in TEK buffer and heated at 88°C for 10 min, then slowly cooled down to room temperature (RT). ATP or cABA was added into the solution and incubated under 37°C for 1h. After the incubation strand R was added into it and incubated for 30 min. At last, G1, G2 and PPIX diluted with TEK buffer were added into the solution and incubated for 60 min before fluorescent test. The fluorescent analysis was performed in the TEK buffer with a final concentration of 1.2 μM for PPIX, 0.16 μM for G1 and G2, 192 μM for ATP and 0.1 μM for the other strands.

Fluorescence spectroscopic analysis

Fluoromax-4 Spectrofluorometer (HORIBA Jobin Yvon, Inc., NJ, USA) was used to collect the fluorescence emission spectra of DNA-PPIX complexes in TEK buffer at RT from 550 to 750nm with the excitation wavelength of 410 nm.

Native polyacrylamide gel electrophoresis (PAGE)

The DNA solutions mixed with 6 × loading buffer (TEK buffer, pH 8.0, 50% glycerol, 0.25% bromphenol blue) were analyzed in 15% native polyacrylamide gel. The DNA strands in these samples were added in the order as shown in Scheme 1. Strands S and M were mixed at first and heated at 88°C for 10 min, then slowly cooled down to RT. Then R and cABA or ATP were added into the corresponding samples and incubated under 37°C for 1h. Concentrations for the DNA strands analyzed by PAGE are all 0.2 μM. ATP is added with a concentration of 3.2 mM. The electrophoresis was done in 1 × TBE (pH 8.0) at a constant voltage of 110V for 1 hour. The gels were scanned by a UV transilluminator after staining with GelRed.

Table S1* Sequences of the oligonucleotides used in this work.

Name	Sequence
G1	5’- TGGGT CTTGACGATG -3’
G2	5’- CTAGACGACA TGGGTAGGGCGGG -3’
S	5’- AGTGAGTCATCGTCAAGTGTCGTCTAG -3’
M	5’- CACTTGACGATGACTCACT ACCTTCCT GGGGGAGTATTGCGG AGGAAGGT -3’
R	5’- AAGGT AGTGAGTCATCGTCAAGTG -3’
cABA	5’-ACCTTCCTCCGCAATACTCCCCC-3’

*The sequences are coloured in the same way as in figures.

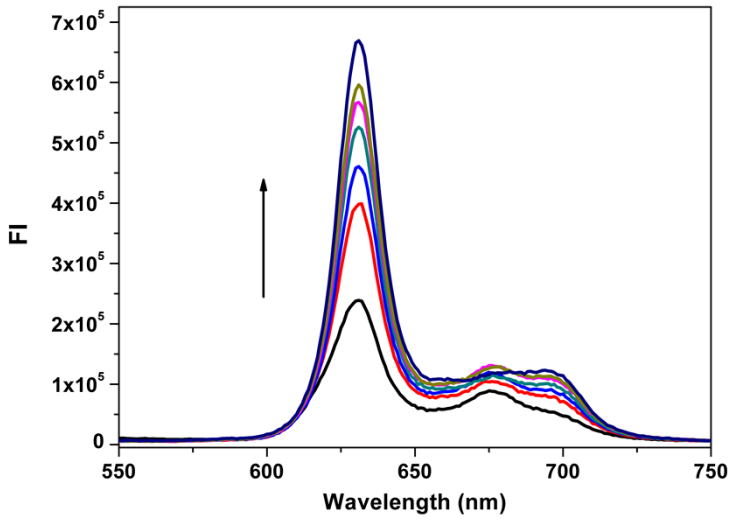

Figure S1. Fluorescence emission spectra of PPIX, G1, G2, S, M, R with different concentrations of ATP (from bottom to top): 0, 32, 64, 96, 128, 160 and 192 μM. The fluorescent analysis was performed in the TEK buffer with a final concentration of 1.2 μM for PPIX, 0.16 μM for G1 and G2 and 0.1 μM for the other strands.

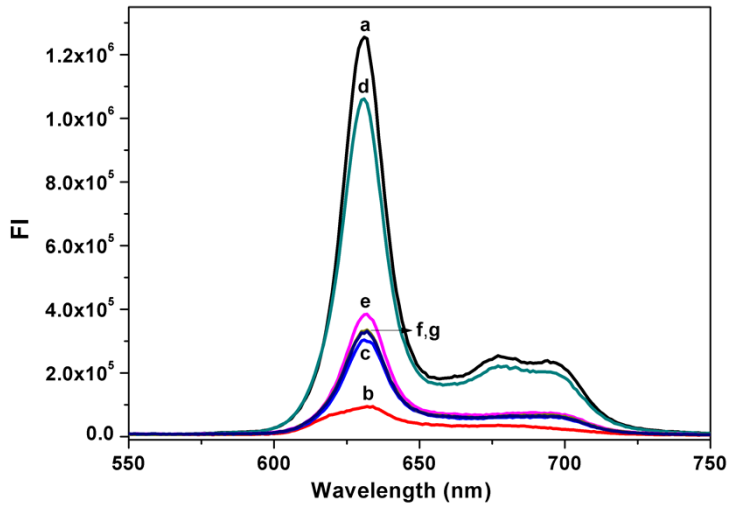

Figure S2. Selectivity of this sensing platform analyzing ATP over CTP, GTP and UTP. PPIX, different DNA strands and small molecules were added in different groups: a) G1, G2, S; b) G1, G2, S, M; c) G1, G2, S, M, R; d) G1, G2, S, M, R, ATP; e) G1, G2, S, M, R, CTP; f) G1, G2, S, M, R, GTP; g) G1, G2, S, M, R, UTP. The spectra were collected in TEK buffer with a final concentration of 1.2 μM for PPIX, 0.16 μM for G1, G2, 0.1 μM for the other strands and 192 μM for ATP, CTP, GTP and UTP.

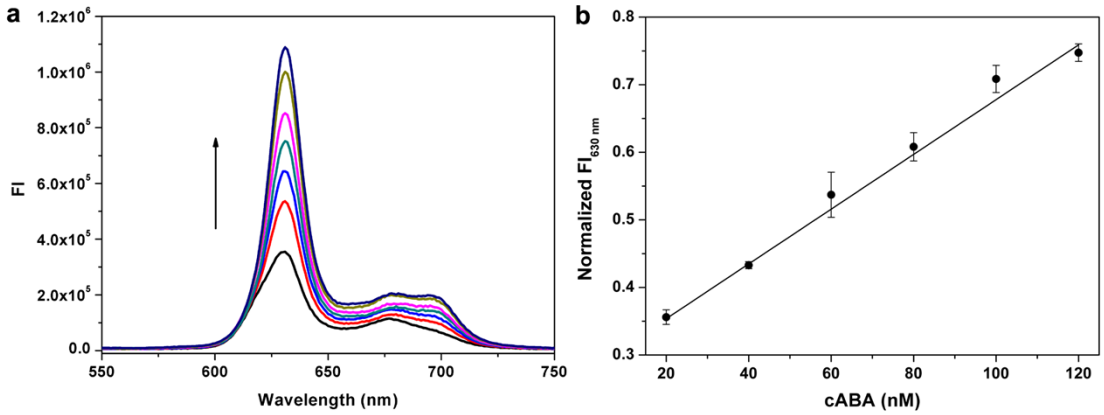

Figure S3. (a) Fluorescence emission spectra of PPIX, G1, G2, S, M, R with different concentrations of cABA (from bottom to top): 0, 20, 40, 60, 80, 100 and 120 nM. The spectra were collected in TEK buffer with a final concentration of 1.2 μM for PPIX, 0.16 μM for G1, G2 and 0.1 μM for the other strands. (b) Dependence of the normalized fluorescence intensity at 630 nm on the cABA concentration from 20 to 120 nM. The data were collected from three independent experiments.

ATP	0	0	1	0	0	1	1	1
cABA	0	1	0	0	1	0	1	1
R	0	0	0	1	1	1	0	1
Output	0	0	0	0	1	1	0	1

Figure S4. Truth table of the logic circuit with three inputs ATP, cABA and R.