Electronic Supplementary Material (ESI) for Analytical Methods
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Supporting information:

Label-free fluorescence turn-on detection of Pb^{2+} based on AIE-active quaternary ammonium salt of 9,10-distyrylanthracene

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Experimental details

Reagents and materials: Nuclease S1 and thrombin-binding aptamer (TBA:5' –GGTTGGTGTGGTTGG - 3') purified by PAGE method were obtained from Sangon Biotechnology Co, Ltd (Shanghai, China). The buffer for nuclease digestion with a pH of 4.6 contained 50 mM sodium acetate and 10 mM Zinc Sulfate and stored at -20°C. The dry crystals of TBA was dissolved in deionized water and then the DNA concentrations were quantified by UV-Vis absorption spectroscopy with the following extinction coefficients (ε_{260nm}, M^{-1} cm^{-1}) for each nucleotide: A = 15400, C = 7400, G

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= 11500, T = 8700. The stock solution of 100 μM TBA stored at 4 °C. The compound 1 (structure shown in Figure 1), which was synthesized according to our previously published procedures, was used as the fluorescence probe in this work. Tris buffer was adjusted to pH 7.2 with acetic acid. Deionized water (18.2 MΩ·cm resistivity) from a Milli-Q water system was used throughout the experiments. The heavy metal salts were prepared in diluted acetic acid to avoid hydrolyzation. All other chemicals were of analytical reagent grade and used without further purification.

Apparatus: UV-vis absorption spectra were recorded using a UV-3600 UV-vis spectrophotometer (Shimadzu, Japan) at room temperature using a 500 μL quartz curette with 1 cm path length. Fluorescence measurements were carried out with 5301PC luminescence spectrometer (Shimadzu, Japan)at room temperature, and the record the fluorescence spectra from 550 to 650 nm with an excitation wavelength at 425 nm. Quartz cuvettes with 1-mm pathlength were used for emission measurements. Circular dichroism spectra were performed with a MOS450 CD spectrometer (Bio-Logic, France) using a 0.5 cm path length cuvette at room temperature. the change in pH value were measured with a FE20 pH meter (Mettler-Toledo, Switzerland).

Fluorescence spectra of compound 1 in the presence of different amounts of TBA: variable amounts of TBA stock solutions (100 μM) were mixed with 25 μL buffer (Tris-HAc, c=200 μM, pH=7.2) in eppendorf cups, then 25 μL compound 1 (50 μM) were mixed with the samples. Subsequently, water was added to eppendorf cups to ensure the total volume of the reaction mixture was 250 μL and the emission spectra

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were recorded at room temperature.

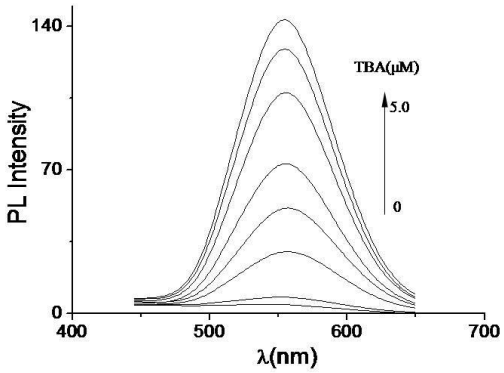

Figure S1. Fluorescence spectra of the compound 1 (5 μM in 20 mM Tris-HAc, pH=7.2) in the presence of different concentrations of thrombin binding aptamer (from 0 to 5.0 μM), λ_{ex}=425 nm.

The absorption spectra of compound 1 in the absence and presence of TBA: 12.5 μL TBA stock solutions (100 μM) were mixed with 25 μL buffer (Tris-HAc, c=200 mM, pH=7.2) in eppendorf cups, then 100 μL compound 1 (50 μM) were mixed with the samples. Subsequently, water was added to eppendorf cups to ensure the total volume of the reaction mixture was 250 μL and the absorption spectra were recorded at room temperature.

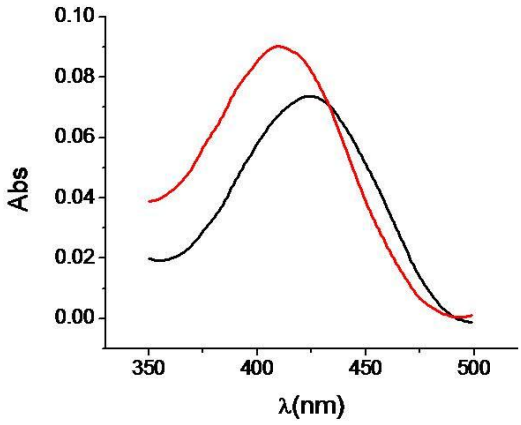

Figure S2. The absorption spectra of compound 1 (20 μM in 20 mM Tris-HAc,

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pH=7.2) in the absence (red line) and presence of TBA (5.0 μM) (black line).

Fluorescence spectrum of compound 1 containing TBA and those after cleavage by nuclease S1 at 37 °C for different time: 12.5 μL of TBA solutions (100 μM) were mixed with 25 μL buffer (Tris-HAc, c=200μM, pH=7.2) in eppendorf cups. Water was added to make the final solution volume of 70 μL. then the samples was heat at 37℃ for 5 minutes, and 10 μL of the nuclease solution (360 U of nuclease S1 + 120 μL of nuclease S1 buffer containing 30 mM CH_3COONa, 280 mM NaCl, and 1 mM ZnSO4, pH 4.6 + 200 μL of water)were added to samples and incubated for different time. The enzymatic digestion was stopped by the addition of 20 μL EDTA (20 mM). Subsequently, the reaction mixtures were cooled to room temperature slowly. Finally, 125 μL water and 25 μL compound 1 (50 μM) were mixed with the samples and the emission spectra were recorded at room temperature.

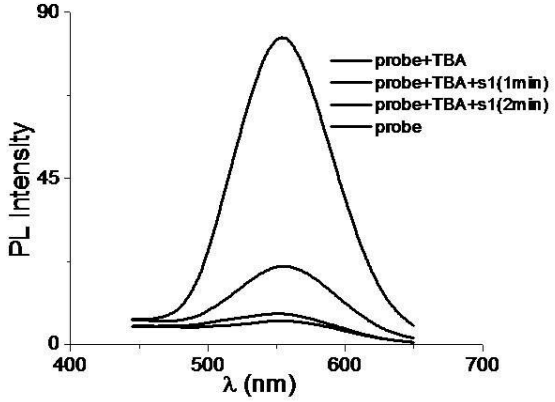

Figure S3. Fluorescence spectra of compound 1 in the different digesting time of Nuclease S1. Experimental conditions: 5.0 μM compound 1, 5.0 μM TBA, 11 U nuclease S1 in 20 mM Tris-HAc, pH=7.2 buffer solution. λ_{ex}=425 nm

Pb^{2+} Assay procedure: 12.5 μL of TBA solutions (100 μM) were mixed with 25 μL

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buffer (Tris-HAc, c=200 μM, pH=7.2) containing different concentrations of Pb^{2+} (acetate salt) in eppendorf cups. Water was added to make the final solution volume of 70 μL. The cups were incubated over eight hours at 26℃ to ensure the TBA switch into G4，then the samples was heat at 37℃ for another 5 minutes, and 10 μL of the nuclease solution (360 U of nuclease S1 + 120 μL of nuclease S1 buffer containing 30 mM CH_3COONa, 280 mM NaCl, and 1 mM ZnSO4, pH 4.6 + 200 μL of water) were added to samples and incubated for 2 min, the enzymatic digestion was stopped by the addition of 20 μL EDTA (20 mM). Subsequently, the reaction mixtures were cooled to room temperature slowly. Finally, 125 μL water and 25 μL compound 1 (50 μM) were mixed with the samples and the emission spectra were recorded at room temperature.