Supporting Information

A sensitive and selective “turn-on” fluorescent probe for Hg\(^{2+}\) based on thymine-Hg\(^{2+}\)-thymine complex with aggregation-induced emission feature

Ke Ma, Xing Li, Bin Xu*, Wenjing Tian*

State Key Laboratory of Supramolecular Structure and Materials, Jilin University, 2699 Qianjin Avenue, Changchun 130012 P. R. China. Fax: +86431 85193421; Tel.: +86431 85168483; xubin@jlu.edu.cn; wjtian@jlu.edu.cn

Table of contents

Experimental Section

Scheme S1. Synthetic route to DSA-T\(_2\)

Figure S1. (A) \(^1\)H NMR spectrum of DSA-T\(_2\) in DMSO-d\(_6\) and (B) \(^1\)H NMR spectrum of DSA-T\(_2\) with the addition of Hg\(^{2+}\) in DMSO-d\(_6\)

Figure S2. TEM image of DSA-T\(_2\) (1.16 × 10\(^{-5}\) mol/L) in CH\(_3\)CN/H\(_2\)O (3:2, v/v) mixture

Experimental Section

Materials and instrumentation.

All reagents and starting materials are commercially available and were used without further purification. Anthracene (99%) was purchased from J&K Chemical Co. (China), 4-tert-Butyibenzaldehyde was purchased from Alfa Aesar Co. (China), 4-Hydroxybenzaldehyde was purchased from Sinopharm Chemical Co. (China), 3,4-Dihydro-2H-pyran (99%) was purchased from Acros (U.S.A), 1,2-Dibromoethane was purchased from Aladdin Chemistry Co. (China), Thymine (>99.0%) was purchased as lyophilized white powders from Shanghai Yuanye Biology Co. (China), all other reagents were purchased as analytical grade from either Tianjin Fuyu Co. (China) or Beijing Chemical Reagent Co. (China). Dimethyl sulfoxide (DMSO) and tetrahydrofuran (THF) were purified by fractional distillation before used as solvents. \(^1\)H NMR spectra were recorded on Bruker AVANCE 600 MHz spectrometer at 298K with deuterated DMSO as solvent and tetramethylsilane (TMS) as the internal standard. Time of flight mass spectra was recorded using a Kratos MALDI-TOF mass system. Fluorescence spectrophotometer was collected on a Shimadzu RF-5301PC spectrophotometer. Transmission electron microscopy (TEM) images were recorded on a JEOL JEM-2100F electron microscope.

Synthesis of DSA-T\(_2\). 9,10-Bis(4-(2-bromoethoxy) styryl) anthracen (DSA-Br\(_2\)) and other compounds were prepared according to literature procedures.\(^{51}\) A round bottomed flask (250 mL) equipped with a magnetic stirring bar was charged with DSA-Br\(_2\) (0.09 g, 0.15 mmol), thymine (0.08 g, 0.63 mmol), K\(_2\)CO\(_3\) (0.22g, 1.60mmol) and DMF (10ml). The flask was then evacuated and charged with nitrogen. The solution was stirred at 60 °C for 72 h. After removing the organic solvents (DMF) with a rotary evaporator, the resultant precipitate was washed with H\(_2\)O for a day and then was washed with CHCl\(_3\) for half a day by using a soxhlet extractor. After evaporating the residue, the yellow powder was achieved as DSA-T\(_2\) (50mg, 50% yield). \(^1\)H NMR (600 MHz, DMSO-D6): \(\delta\) (TMS, ppm): 11.324 (s, 2H), 8.368-8.384 (m, 4H), 7.963-7.990 (d, J=16.2Hz, 2H), 7.749-7.763 (d, J=8.4Hz, 4H), 7.610 (m, 2H), 7.537-7.552 (m, 4H), 7.036-7.050 (d, J=8.4Hz, 4H), 6.854-6.882 (d, J=16.8Hz, 2H), 4.256 (t, 4H), 4.063 (t, 4H), 1.792 (s, 6H). MALDI/TOF MS calcd for DSA-T\(_2\): 718.28, Found: 718.185. Anal. calcd for DSA-T\(_2\): C, 73.52; H, 5.33; N, 7.79. Found: C, 73.50; H, 5.36; N, 7.76.
**Scheme S1.** Synthetic route to DSA-T$_2$

Reference

Figure S1. (A) $^1$H NMR spectrum of DSA-T$_2$ in DMSO-d$_6$ and (B) $^1$H NMR spectrum of DSA-T$_2$ with the addition of Hg$^{2+}$ in DMSO-d$_6$. 
Figure S2. TEM image of DSA-T$_2$ (1.16 × 10$^{-5}$ mol/L) in CH$_3$CN/H$_2$O (3:2, v/v) mixture