Electronic Supplementary Material (ESI) for Polymer Chemistry.

Electronic Supplementary Information

Selective visualization of endogenous hydrogen sulfide in lysosomes via using aggregation induced emission dots

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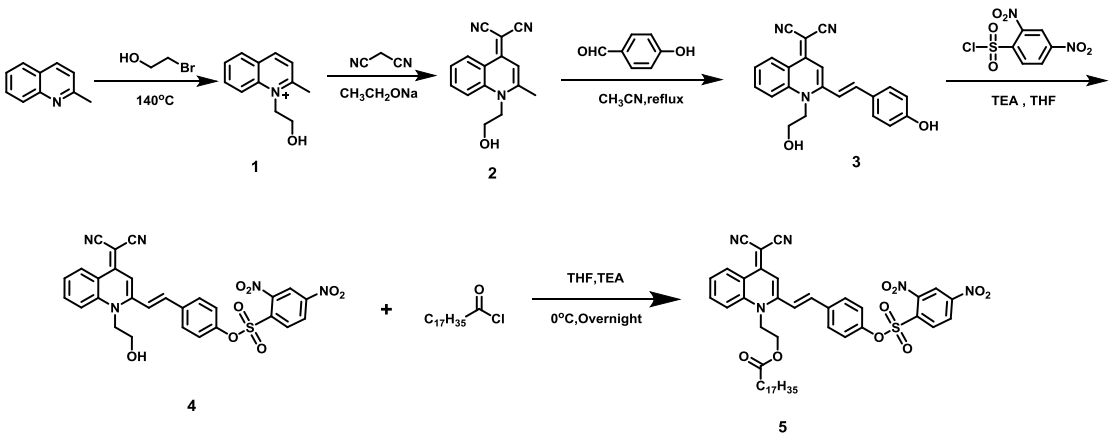
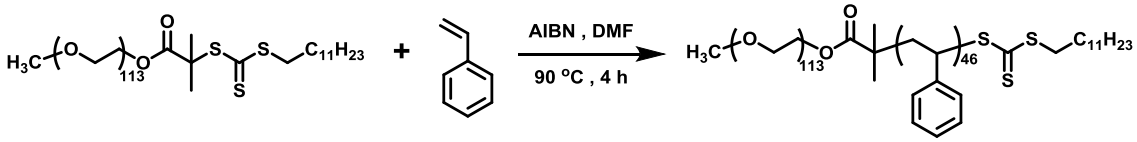


Scheme S1. Synthesis route of compound **5**



Scheme S2. Synthesis route of **PEO_{113}-*b*-PS_{46}**.

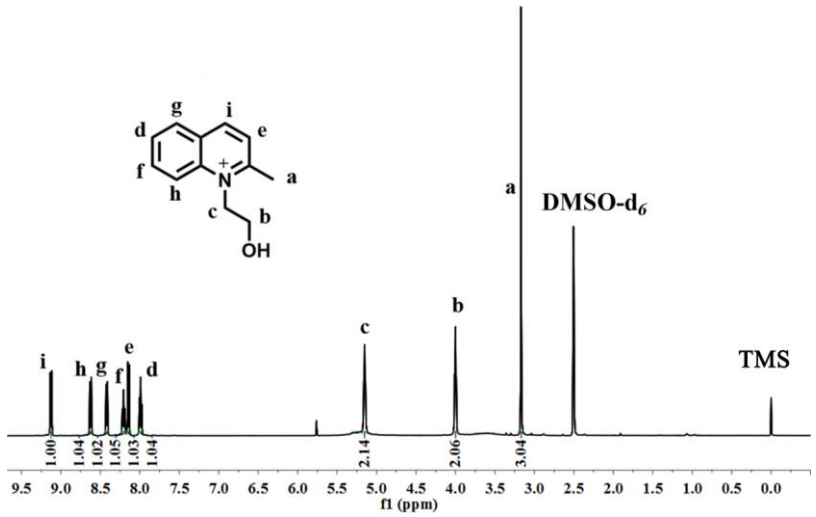


Figure S1 ^{1}H NMR spectrum (in DMSO-d_6) of the compound **1**.

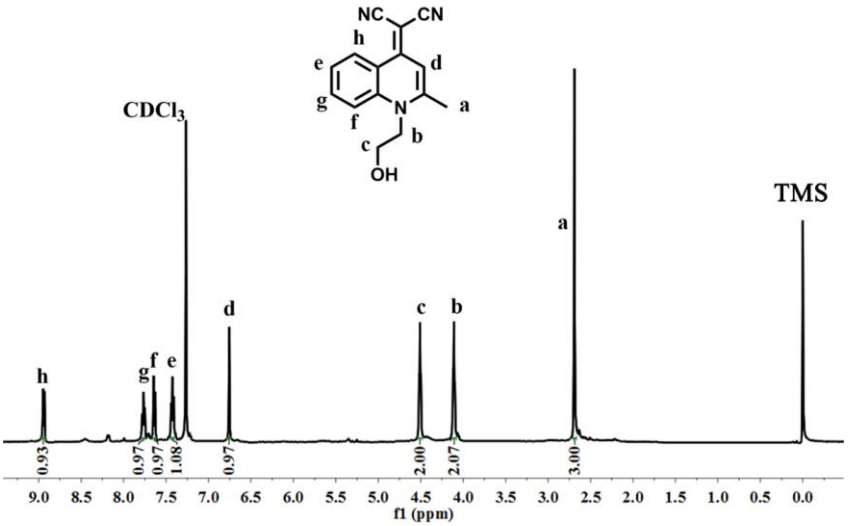


Figure S2 ^{1}H NMR spectrum (in $CDCl_3$) of the compound **2**.

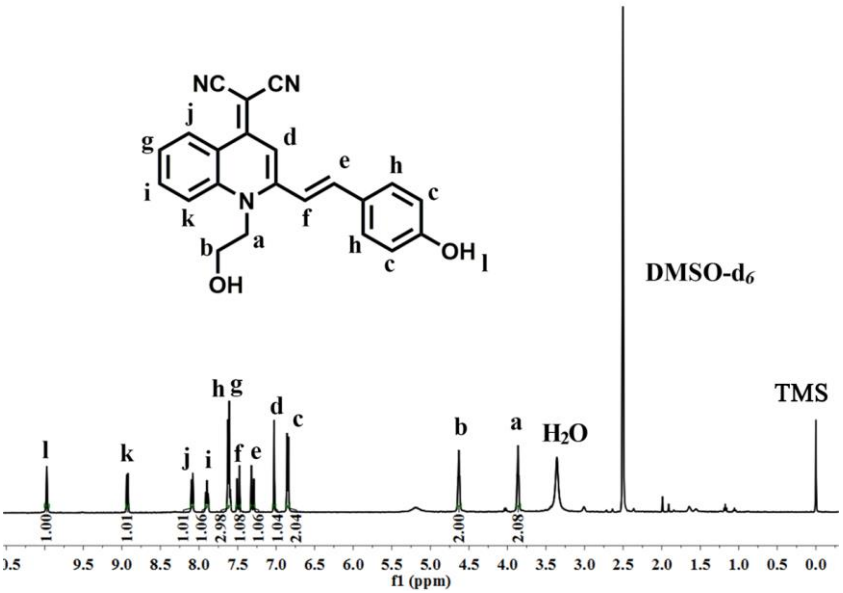


Figure S3 ^{1}H NMR spectrum (in DMSO-d_6) of the compound **3**.

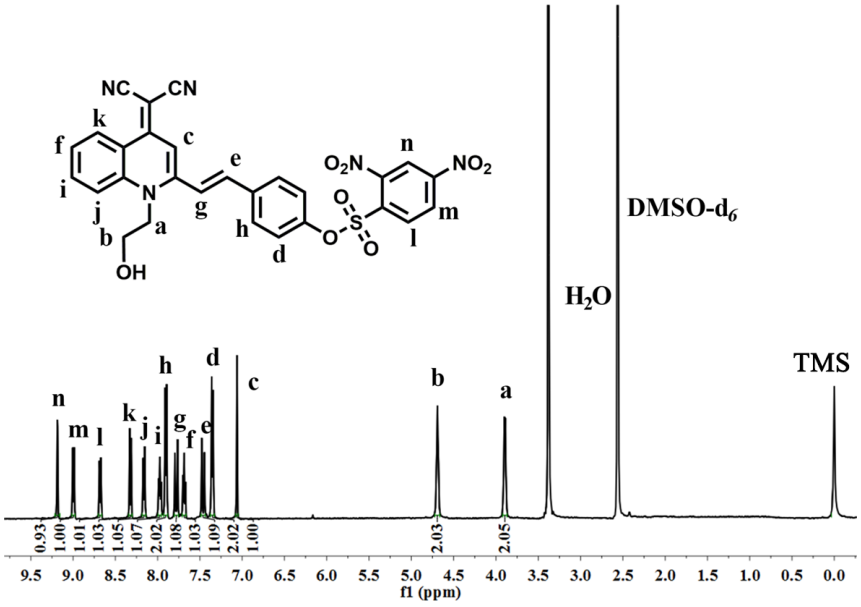
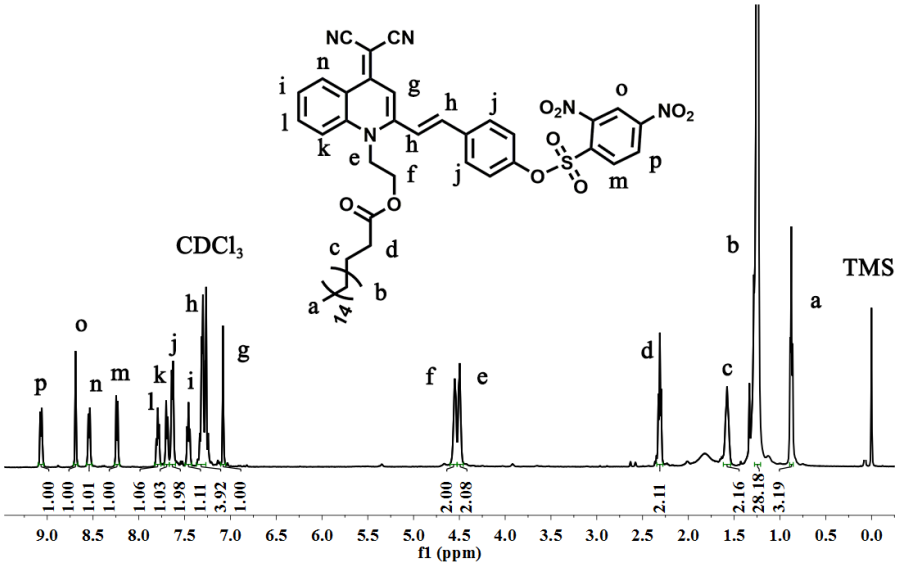
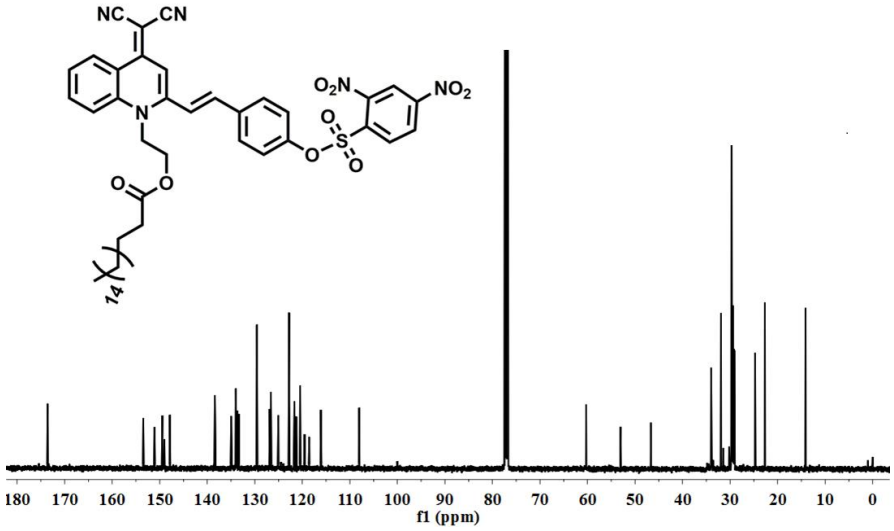


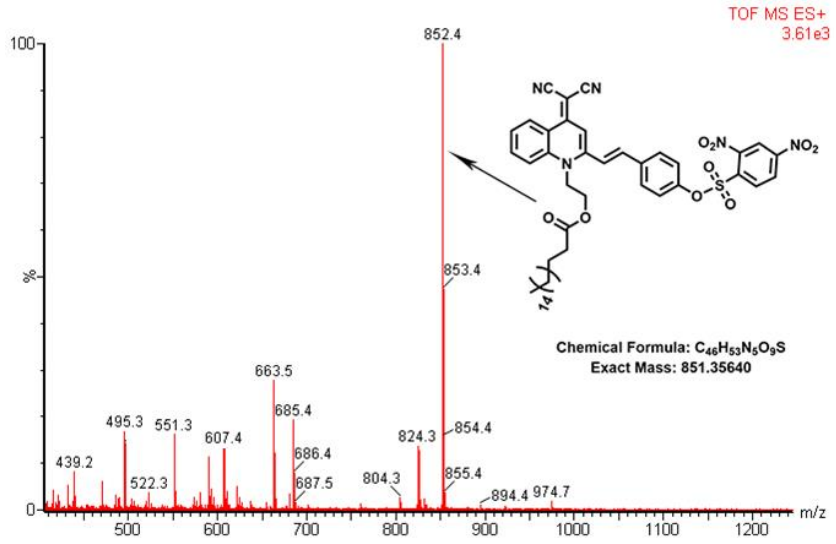
Figure S4 ^{1}H NMR spectrum (in DMSO-d_6) of the compound **4**.



(A)



(B)



(C)

Figure S5 (A) ^{1}H NMR (in $CDCl_3$), (B) ^{13}C NMR and (C) Mass spectrum of the compound **5**.

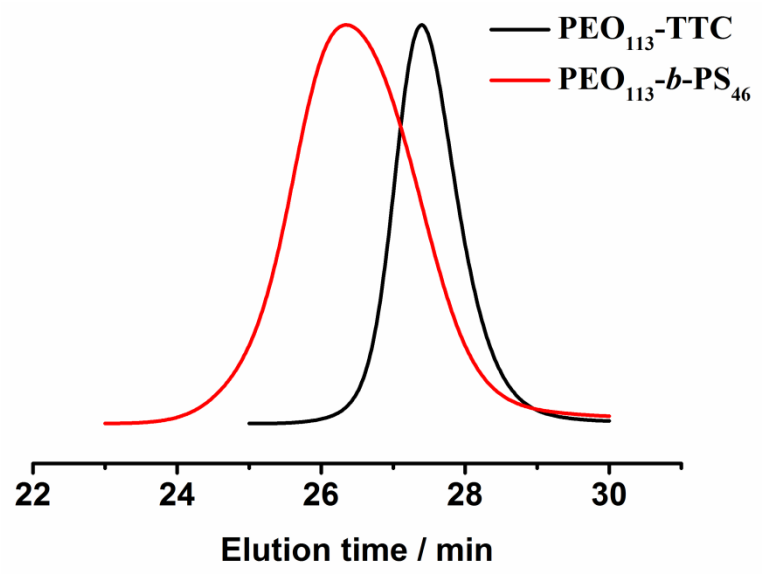


Figure S6. GPC trace of **PEO_{113}-TTC** and **PEO_{113}-*b*-PS_{46}**.

Table S1. Molecular weight distribution data of starting linear polymers

Sample	$M_{n,GPC}$[a]	$M_{w,GPC}$[a]	PDI
PEO_{113}-TTC	8206	8699	1.06
PEO_{113}-*b*-PS_{46}	13125	15380	1.17

[a]The data were acquired using SEC based on a polystyrene calibration curve and obtained from GPC analysis was using THF as eluent at a flow rate of 1.0 mL/min.

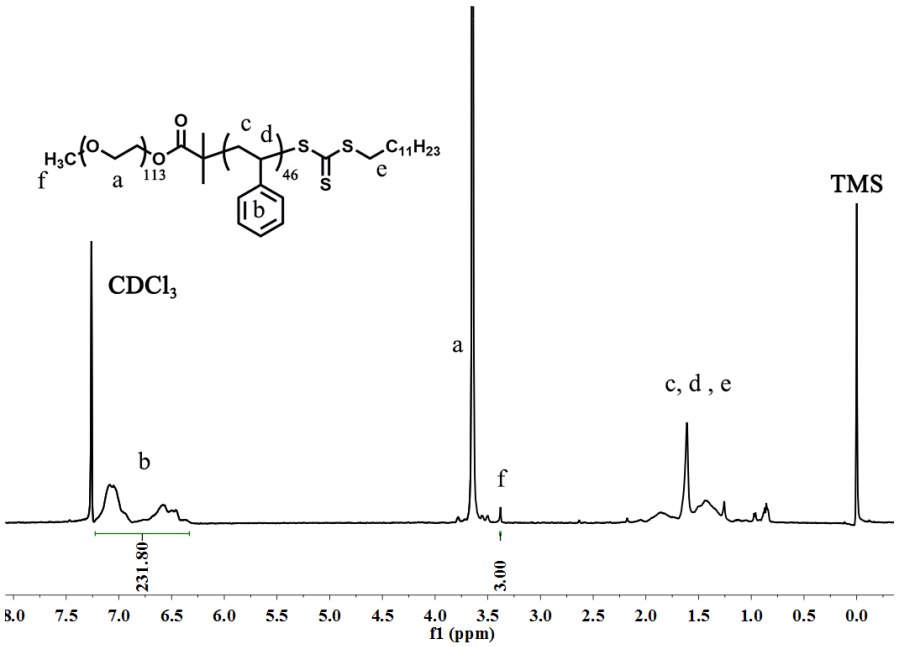


Figure S7. ^{1}H-NMR spectrum (in $CDCl_3$) of **PEO_{113}-*b*-PS_{46}**.

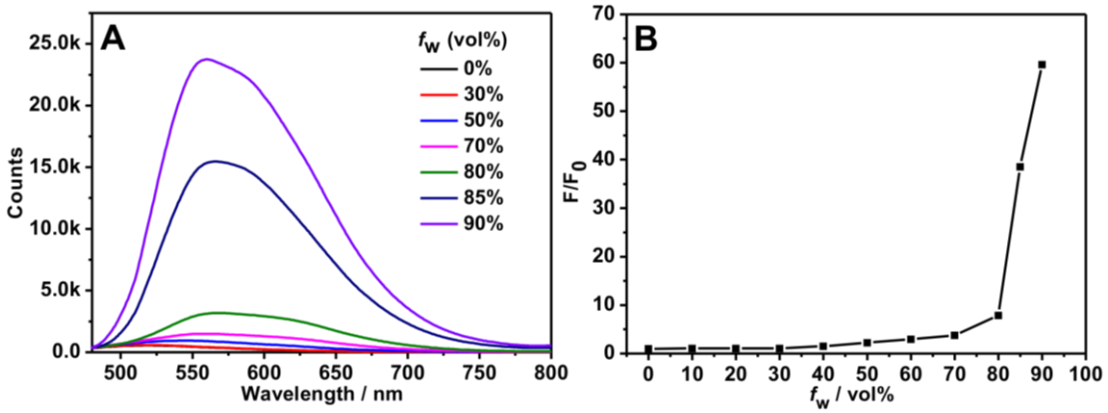


Figure S8. (A) Fluorescence emission spectra of compound **3** in water/THF mixtures with varied water fractions, λ_{ex} = 435 nm. (B) Compound **3** with f_w. F_0 and F are the PL intensities in THF (f_w = 0) and a THF/water mixture with a specific f_w, respectively.

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Determination of fluorescence quantum yield of the compound 3

The quantum yield can be described as follows:

$$\Phi_U = \Phi_S \times \frac{F_U}{F_S} \times \frac{A_S}{A_U} \times \frac{(n_U)^2}{(n_S)^2}$$

Where Φ_s is the fluorescence quantum yield of the standard (rhodamine B in ethanol, 65%, 25 ℃)[1], F_U and F_S are the integral area of fluorescence intensity of the unknown sample and the standard at the same excitation wavelength, respectively; A_U and A_S are the absorbance of the unknown sample and the standard at the defined excitation wavelength, respectively; n_S and n_U are the refractive index at 25 ℃ of the solvent of standard (ethanol) and the unknown sample (mainly H_2O), respectively.

The Φ_U of compound 3 was calculated to be 2.8%.

[1]. R.F. Kubin, A.N. Fletcher, *J. Lumin.* **1982**, *27*, 455-462

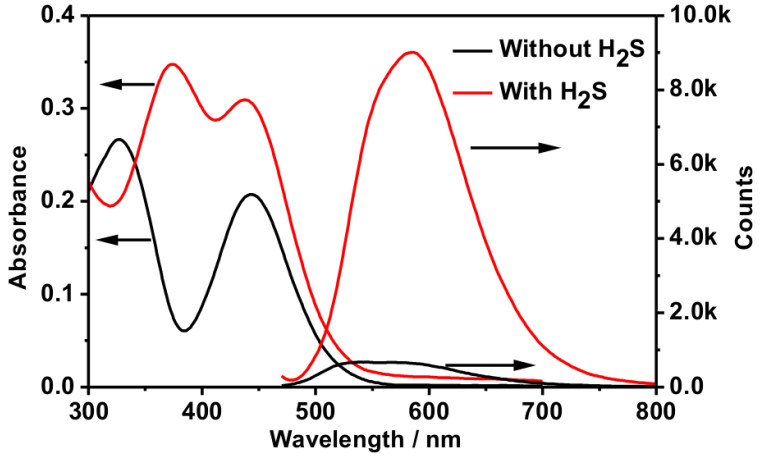


Figure S9. Absorbance and fluorescence spectra of **AIED** (10 μg/mL) in pH 5.0 PBS buffered water without (black) and with (red) H_2S (80 μM), λ_{ex} = 435 nm.

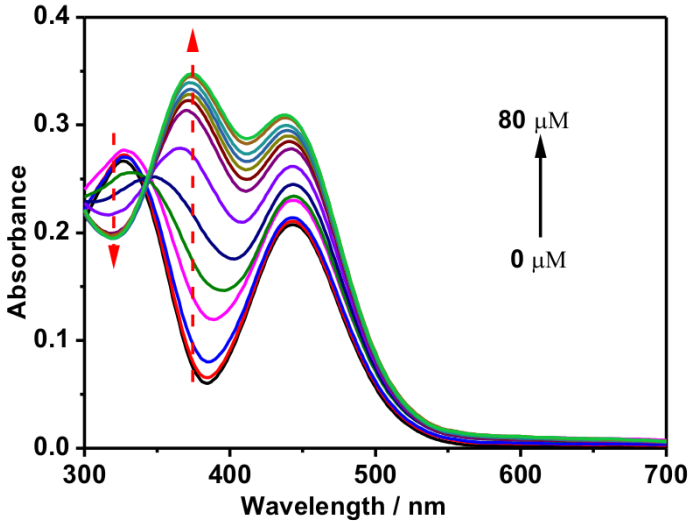


Figure S10. Absorbance spectra of **AIED** (10 μg/mL) in pH 5.0 PBS buffered water under different concentration of H_2S (0~ 80 μM).

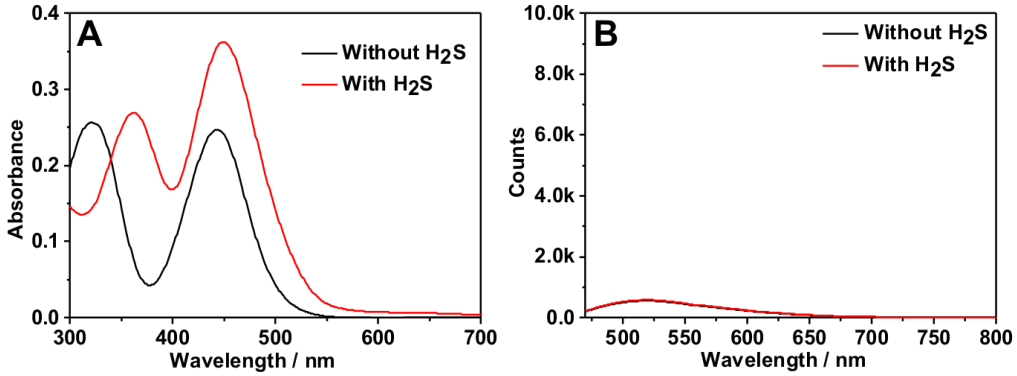


Figure S11. Absorbance (A) and fluorescence spectra (B) of compound 5 in pure THF without (black) and with (red) H_2S (80 μM), λ_{ex} = 435 nm.

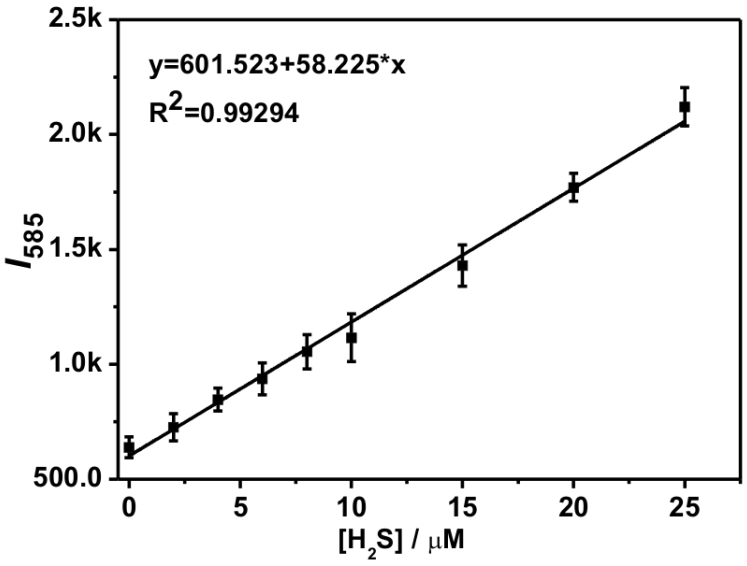


Figure S12. Linear relationship curve of fluorescence intensity at 585 nm (I_{585}) versus concentration of H_2S (0 ~ 25 μM), λ_{ex} = 435 nm.

Determination of the detection limit:

First the calibration curve was obtained from the plot of fluorescence intensity (I_{585}) versus H_2S concentration. The regression curve equation was then obtained for the lower concentration part.

The detection limit = 3 ×S.D. / k

Where k is the slope of the curve equation, and S.D. represents the standard deviation for the fluorescence intensity (I_{585}) of **AIED** in the absence of H_2S.

I_{585}= 601.523 + 58.225×[H_2S] (R^2 =0.9929)

LOD = 3 × 0. 8494 /58.225 = 0.0438 μM = 43.8 nM.

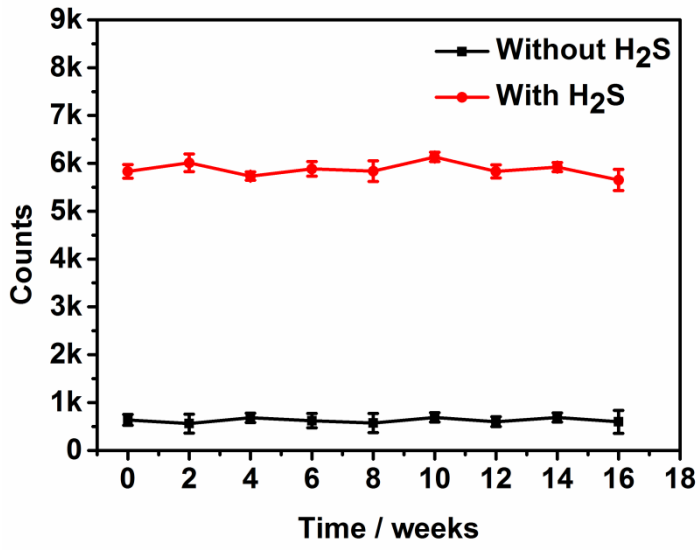
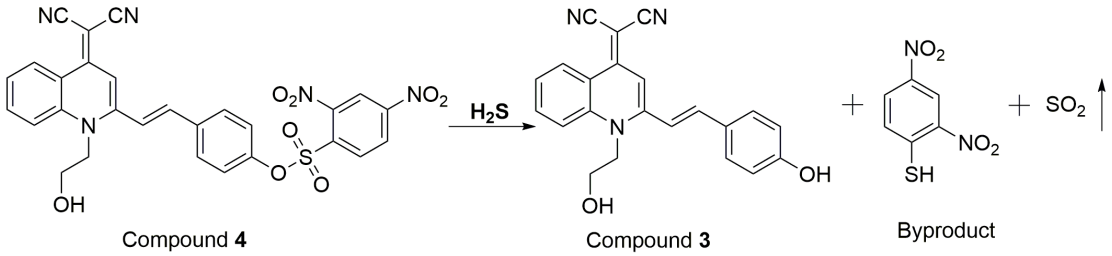
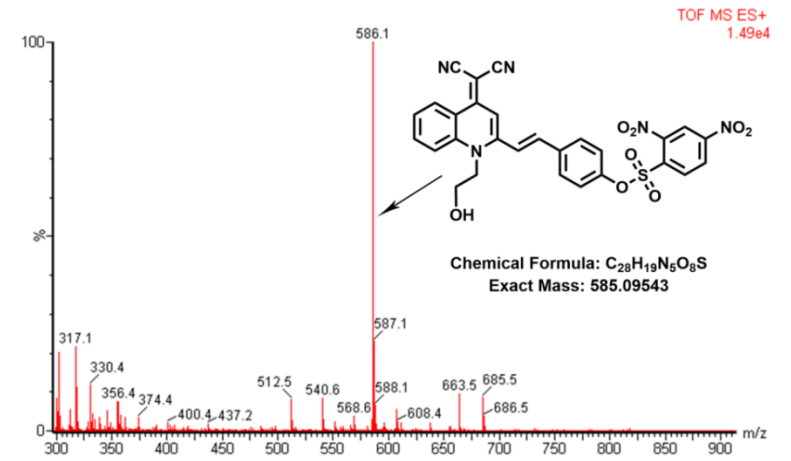


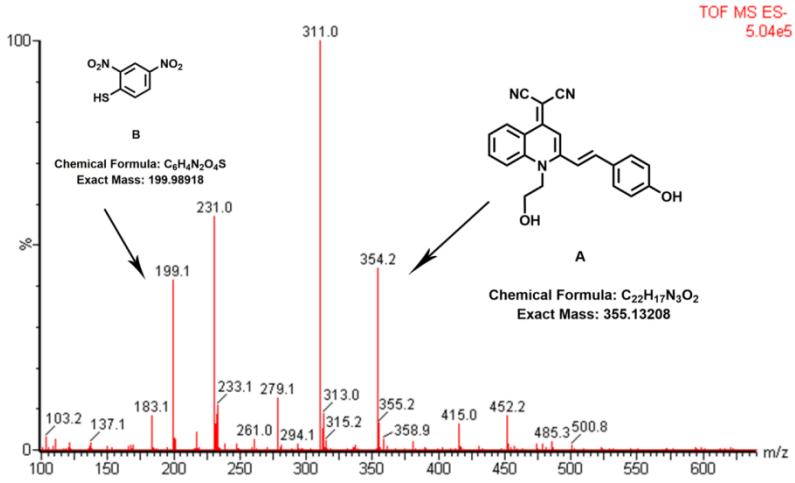
Figure S13. Fluorescence long-term photostability of **AIED** (10 μg/mL) at 585 nm (I_{585}) without and with H_2S (80 μM). λ_{ex} = 435 nm.



Scheme S3. Possible reaction mechanism of compound **4** with H_2S;



(A)



(B)

Figure S14. Mass spectra of compound **4** before (A) and after (B) addition H_2S. For A: the signals at m/z 586.1 are [(compound **4**)+H]$^+$; For B: the signals at m/z 199.1, 231.0 and 354.2 are [(Byproduct)-H]$^-$, [(Byproduct)+CH_3OH-H]$^-$ and [(compound **3**)-H]$^-$, respectively.

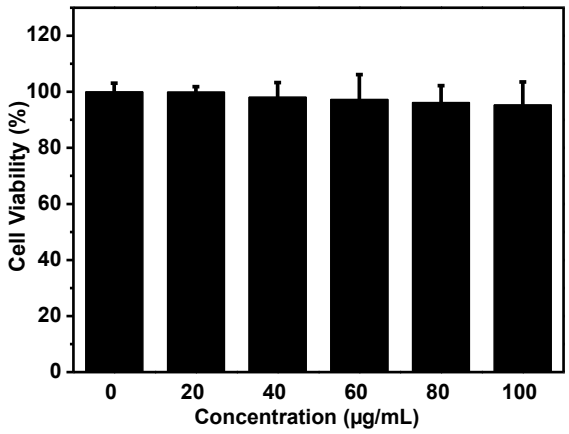


Figure S15. Viability for HeLa cells treated with the varied concentrations of **AIED** for 24 h.

Table S2. Comparison of the recently reported H_2S fluorescent probes

Probes	Solution	Detection limit/nM	Stokes shift	AIE characteristics	Reference
HSN2-BG	PBS	--	109 nm	No	Anal. Chem., 2016, 88, 5769-5774.
Lyso-HS	PBS buffer (pH 7.4, 1% DMSO)	--	120 nm	No	Anal. Chem., 2016, 88, 9213-9218.
SulpHensor	Buffer solution (pH 4.5, 10% DMF,)	--	25 nm	No	Anal. Chem., 2014, 86, 7508-7515.
Lyso-NHS	PBS buffer (pH 7.4, 10% CH_3CN)	480 nM	105 nm	No	Org. Lett., 2013, 15, 2310-2313
Lyso-AFP	HEPES buffer (pH 7.4, 50% CH_3CN)	--	109 nm	No	RSC Adv., 2014, 4, 25790-25794.
1	CTAB 1.0 mM, CH_3CN / Tris-HCl = 3 : 7, pH = 7.4	790 nM	138 nm	No	Chem. Commun., 2014, 50, 13833-13836.
TP-PMVC	PBS buffer (pH 4.4, 5% DMSO)	--	70 nm	No	Chem. Commun., 2016, 52, 7016-7019
AIED	PBS buffer (pH 5.0,)	43.8 nM	150 nm	Yes	This work