Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information

A PEGylated colorimetric and turn-on fluorescent sensor based on BODIPY for Hg(II) detection in water

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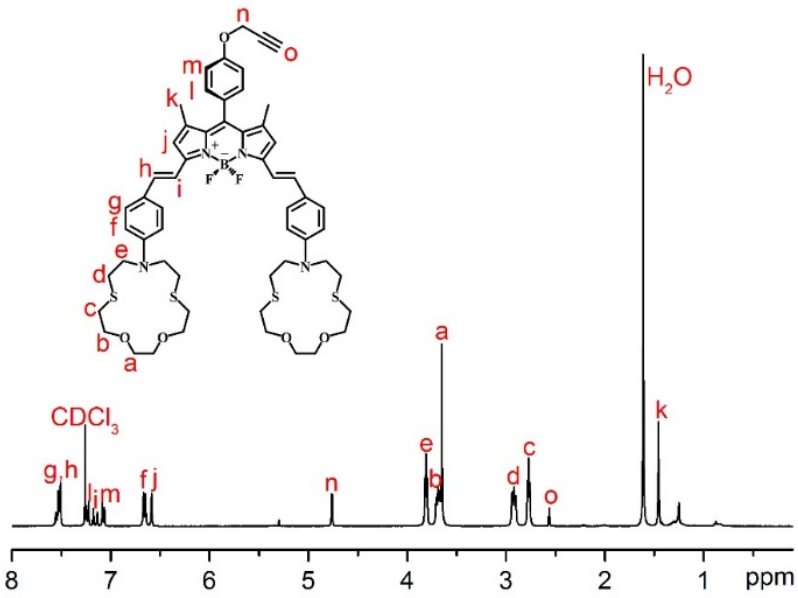


Fig. S1. ^{1}H NMR spectrum of compound DMS1 in $CDCl_3$.

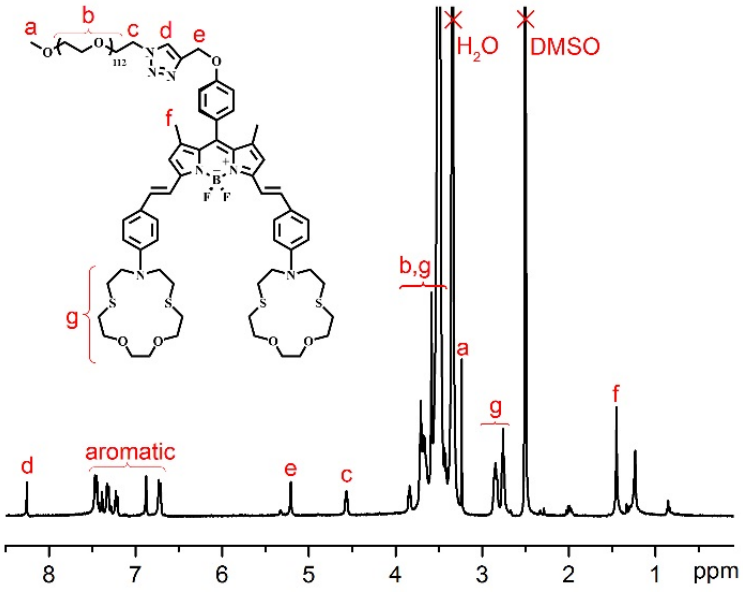


Fig. S2. ^{1}H NMR spectrum of PEG-DMS2 in DMSO-d_6.

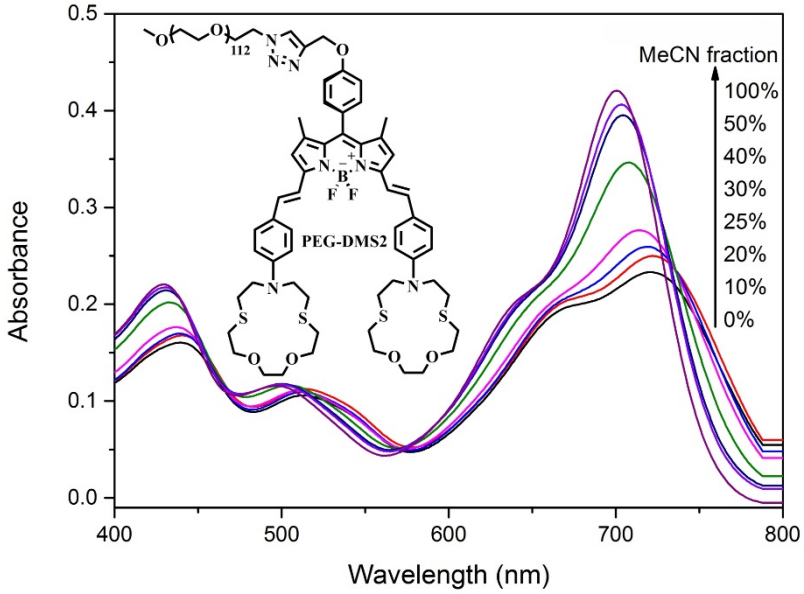


Fig. S3. UV-Vis spectra of 5 μM PEG-DMS2 in MeCN/water mixtures with different MeCN fractions.

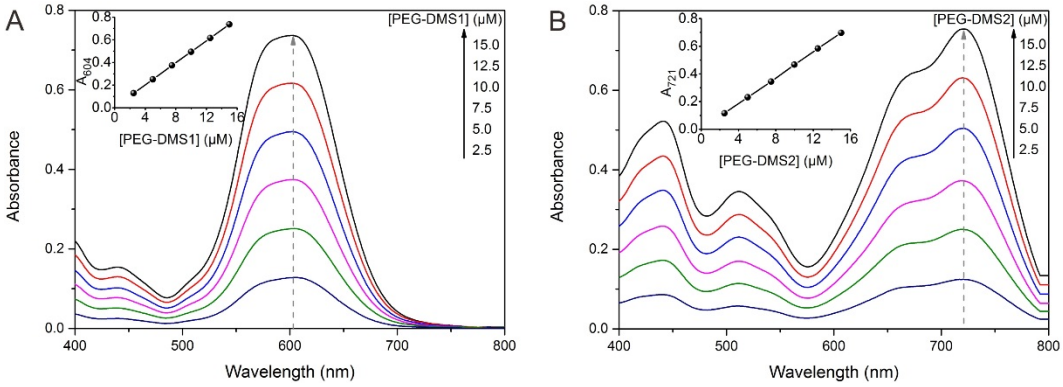


Fig. S4. UV-Vis spectra of PEG-DMS1 (A) and PEG-DMS2 (B) in pure water at different concentrations. Insets: the Q-band absorbance vs. the concentration of PEG-DMS.

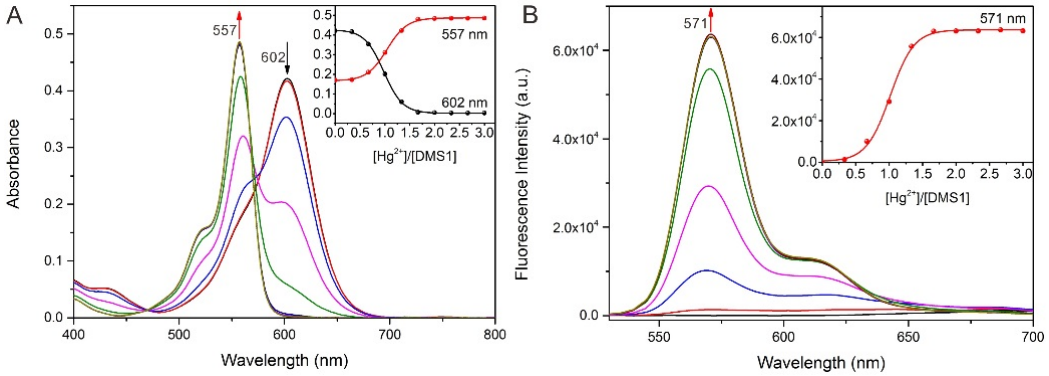


Fig. S5. UV-Vis (A) and fluorescence (B) titration of 5 μM DMS1 with Hg^{2+} (3 equiv.) in MeCN. Insets: absorbance (inset A) and fluorescence (inset B) intensity as a function of the molar ratio ($[Hg^{2+}]/[DMS1]$).

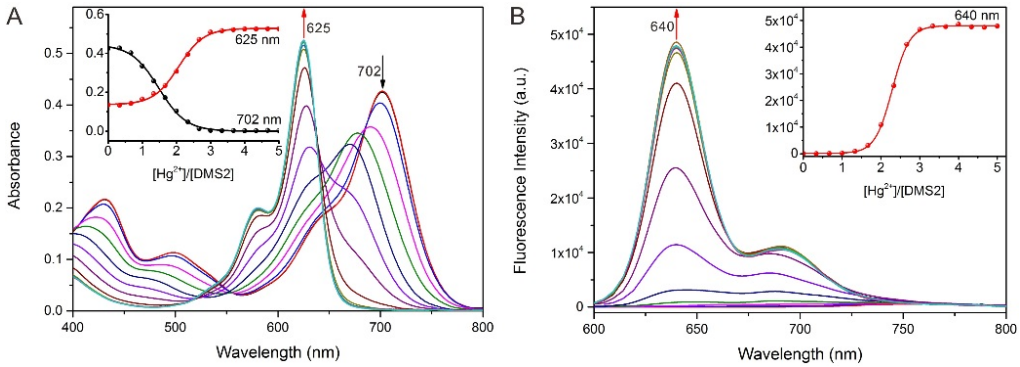


Fig. S6. UV-Vis (A) and fluorescence (B) titration of 5 μM DMS2 with Hg^{2+} (5 equiv.) in MeCN. Insets: absorbance (inset A) and fluorescence (inset B) intensity as a function of the molar ratio ($[Hg^{2+}]/[DMS2]$).

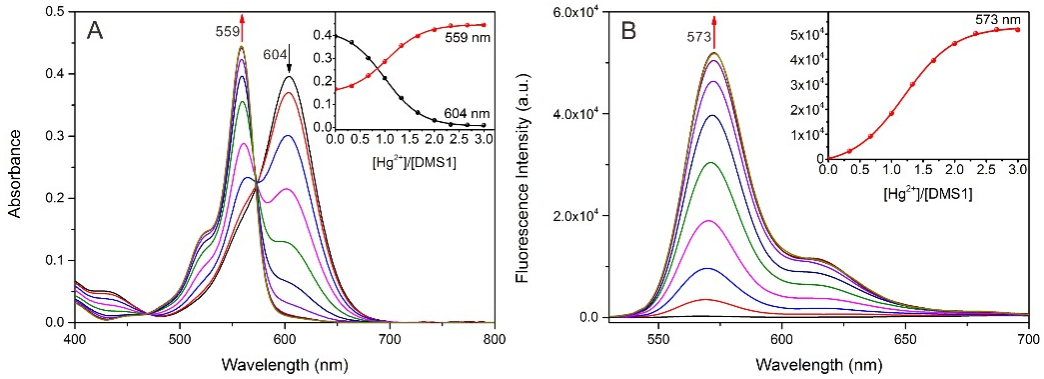


Fig. S7. UV-Vis (A) and fluorescence (B) titration of 5 μM DMS1 with Hg^{2+} (3 equiv.) in a MeCN-H_2O mixture (5/5, v/v). Insets: the absorbance (inset A) and fluorescence (inset B) intensity as a function of the molar ratio ([Hg^{2+}]/[DMS1]).

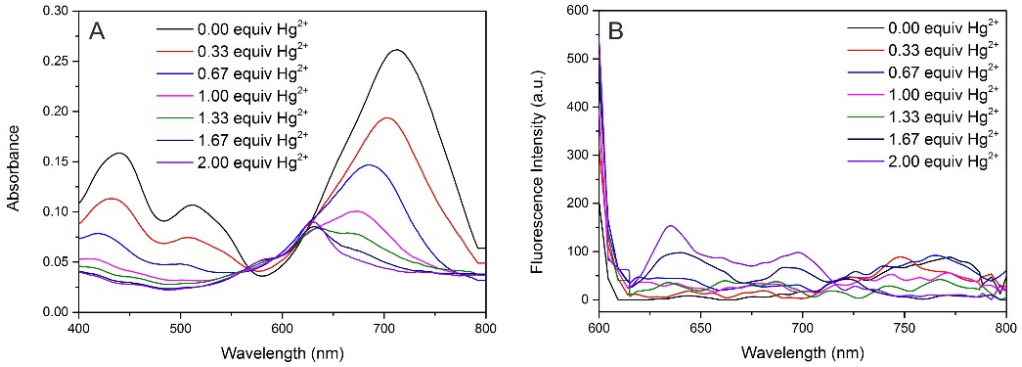


Fig. S8. UV-Vis (A) and fluorescence (B) titration of 5 μM DMS2 with Hg^{2+} (2 equiv.) in a MeCN-H_2O mixture (5/5, v/v).

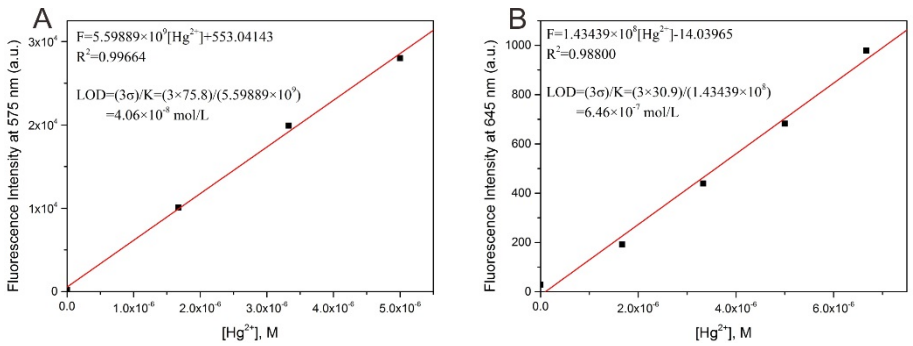


Fig. S9. The fluorescence intensity of PEG-DMS (5 μM) as a function of Hg^{2+} concentration in water. (A) PEG-DMS1, Hg^{2+} concentration: 0 – 5 μM, λ_{ex} = 510 nm; (B) PEG-DMS2, Hg^{2+} concentration: 0 – 6.67 μM, λ_{ex} = 590 nm.

The method for determining the limit of detection (LOD):[1]

LOD = 3σ/*K*, σ: standard deviation from the blank measurement in the absence of Hg^{2+}; *K*: slope of the calibration plot.

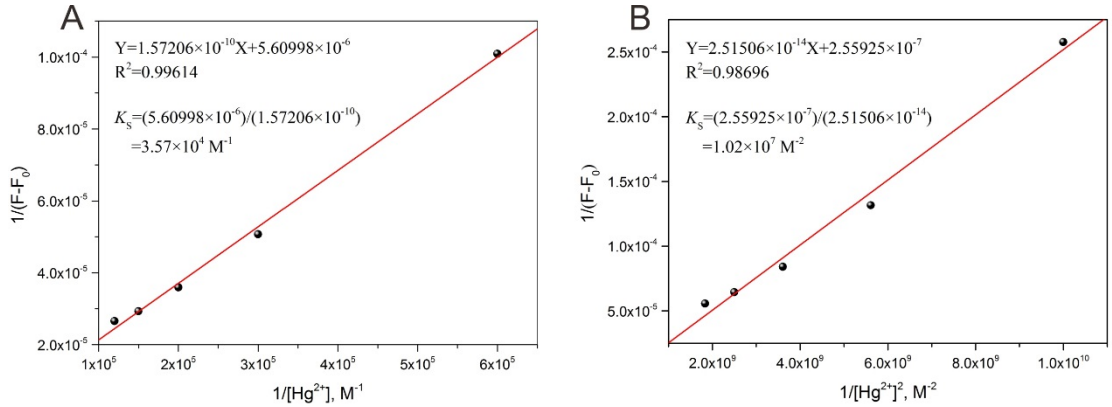


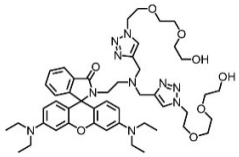
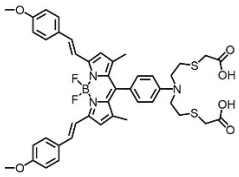
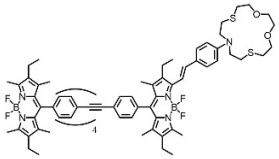
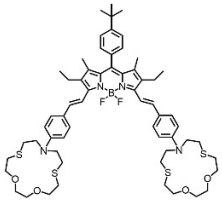
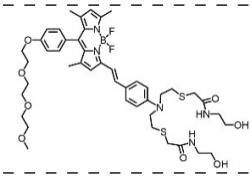
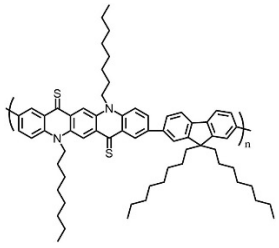
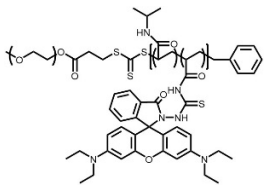
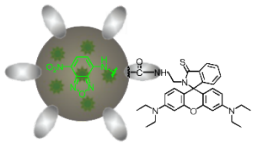
Fig. 10. Benesi-Hildebrand plot of PEG-DMS with Hg^{2+}. (A) PEG-DMS1; (B) PEG-DMS2.

The method for determining stability constant (K_s) via Benesi-Hildebrand plot:[2]

$$\frac{1}{F - F_{min}} = \frac{1}{F_{max} - F_{min}}[1 + \frac{1}{K_s[X]^n}]$$

F: fluorescence intensity at λ_{em}; F_{min} and F_{max} denote the fluorescence signals at minimal [X] and maximal [X]; [X]: analyte concentration; n: stoichiometry of binding.

Table S1. Comparison of the properties of PEG-DMS with those literatures reported.

Probes	$\lambda_{ex}/\lambda_{em}$ (nm)	Detection medium	Limit of detection
	530/580	water	2.3 ppb[1]
	370/655	MeCN : HEPES buffer (1:1, v/v)	3 ppb[2]
	500/600	THF	not reported[3]
	640/655	THF	not reported[4]
	510/572	MeCN : water (2:3, v/v)	not reported[5]
	380/566	PBS solution to obtain nanoparticles	<1 ppb[6]
	500/584	water	3.5 ppb at 25℃[7] 1.6 ppb at 40℃
	420/593	HEPES buffer pH = 7.0	20 ppb[8]
PEG-DMS1	510/575	water	8.1 ppb

PEG-DMS2	590/645	129.3 ppb

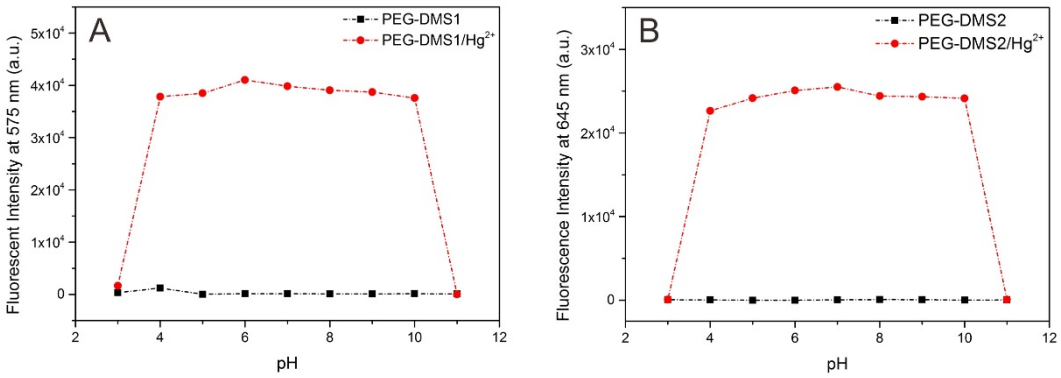


Fig. S11. Fluorescence intensity of PEG-DMS (5 μM) in water at different pH both in the absence and presence of Hg^{2+}. (A) PEG-DMS1, 5 equiv. of Hg^{2+}, λ_{ex} = 510 nm; (B) PEG-DMS2, 10 equiv. of Hg^{2+}, λ_{ex} = 590 nm.

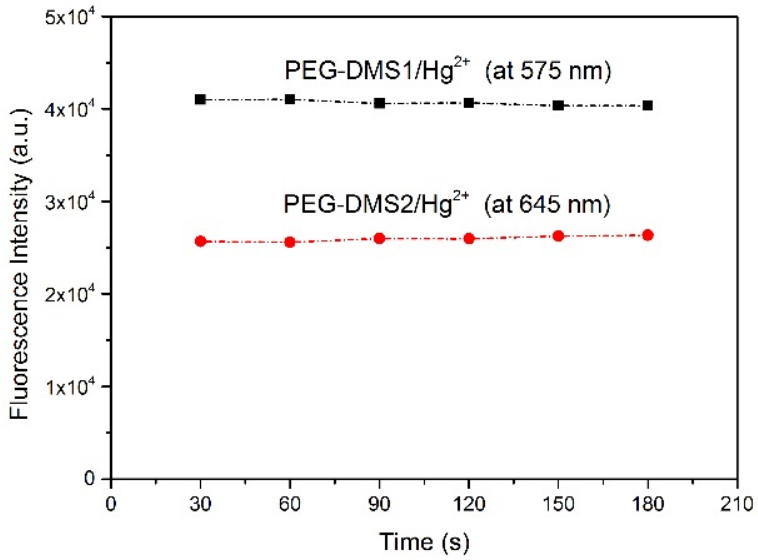


Fig. 12. Time-dependent fluorescence intensity of PEG-DMS (5 μM) upon addition of Hg^{2+}. 5 equiv. of Hg^{2+} for PEG-DMS1 (λ_{ex} = 510 nm); 10 equiv. of Hg^{2+} for PEG-DMS2 (λ_{ex} = 590 nm).

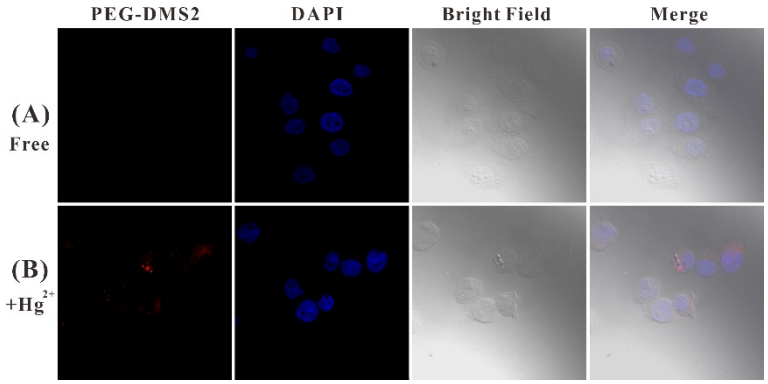


Fig. 13. CLSM images of HeLa cells incubated within 20 μM of PEG-DMS1 for 12 h before (A) and after (B) being treated 20 μM of Hg^{2+} for 0.5 h. The images from left to right were PEG-DMS1 fluorescence (emission collected at 620 – 730 nm upon λ_{ex} = 633 nm), nuclei staining with DAPI (emission collected at 425 – 475 nm upon λ_{ex} = 405 nm), bright field and overlays of images.

References

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