Electronic Supplementary Information (ESI)

Novel “turn-on” fluorescent chemodosimeters based on thioxanthen-9-thione for the selective detection of mercuric ion in aqueous media

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Figure S1. $^1$H NMR (400 MHz, CDCl$_3$) spectrum of compound DB-TXO.
Figure S2. ESI-MS spectrum of compound DB-TXO.

Figure S3. $^1$H NMR (400 MHz, CDCl$_3$) spectrum of compound DP-TXO.
Figure S4. $^{13}$C NMR (100 MHz, CDCl$_3$) spectrum of compound DP-TXO.

Monoisotopic Mass, Even Electron ions
217 formula(s) evaluated with 188 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-80  H: 0-160  O: 0-16  S: 0-3

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Figure S5. ESI-MS spectrum of compound DP-TXO.
Figure S6. $^1$H NMR (400 MHz, CDCl$_3$) spectrum of compound DP-TXT.

Figure S7. $^{13}$C NMR (100 MHz, CDCl$_3$) spectrum of compound DP-TXT.
Figure S8. ESI-MS spectrum of compound DP-TXT.

Figure S9. $^1$H NMR (400 MHz, DMSO-$d_6$) spectrum of compound BDPA-TXO.
Figure S10. $^{13}$C NMR (100 MHz, CDCl$_3$) spectrum of compound BDPA-TXO.

Figure S11. ESI-MS spectrum of compound BDPA-TXO.
Figure S12. $^1$H NMR (400 MHz, DMSO-$d_6$) spectrum of compound BDPA-TXT.

Figure S13. $^{13}$C NMR (100 MHz, CDCl$_3$) spectrum of compound BDPA-TXT.
Figure S14. ESI-MS spectrum of compound BDPA-TXT.

Figure S15. A plot of fluorescence intensity change of DP-TXT (10.0 μM) against varied concentrations of Hg²⁺ (5.0–30.0 μM) in CH₃CN–H₂O (5:5, v/v) (λₑₓ = 309 nm, slit: 5 nm/5 nm, PMT Volts: 610.). R² = 0.9934, k = 3.7×10⁷ au/M. The Standard deviation (σ = 0.26) was obtained by fluorescence responses (10-times of consecutive scanning on the Varian Cary Eclipse Fluorescence Spectrophotometer). Therefore, the detection limit was calculated by the formula (3σ/k) and gave a result 21 nM.
**Figure S16.** Partial $^1$H NMR spectrum (400 MHz, CDCl$_3$) of chemodosimeter DP-TXT before and after addition of excessive Hg$^{2+}$

**Figure S17.** Partial $^1$H NMR spectrum (400 MHz, DMSO-$d_6$) of chemodosimeter BDPA-TXT before and after addition of excessive Hg$^{2+}$
Figure S18. A plot of fluorescence intensity change of BDPA-TXT (10.0 μM) against varied concentrations of Hg\(^{2+}\) (5.0–40.0 μM) in DMSO–H\(_2\)O (9:1, v/v) (λ\(_{\text{ex}}\) = 357 nm, slit: 5 nm/5 nm, PMT Volts: 800.), \(R^2 = 0.9944\), \(k = 1.2 \times 10^7\) au/M. The Standard deviation (σ = 0.30) was obtained by fluorescence responses (10-times of consecutive scanning on the Varian Cary Eclipse Fluorescence Spectrophotometer). Therefore, the detection limit was calculated by the formula (3σ/k) and gave a result 75 nM.
**Figure S19.** HRMS (ESI) spectra of compound BDPA-TXT in the absence and in the presence of Hg$^{2+}$.
**Figure S20.** HRMS (ESI) spectra of compound DP-TXT in the absence and in the presence of Hg$^{2+}$.

**Figure S21.** (a) Emission ratiometric response of DP-TXT to various metal ions. [DP-TXT] = 1.0×10$^{-5}$ M, [Hg$^{2+}$] = 3.0×10$^{-5}$ M, [M$^{n+}$] = 1.0×10$^{-4}$ M. (b) Emission ratiometric response of BDPA-TXT to various metal ions. [BDPA-TXT] = 1.0×10$^{-5}$ M, [Hg$^{2+}$] = 4.0×10$^{-5}$ M, [M$^{n+}$] = 1.0×10$^{-4}$ M.