

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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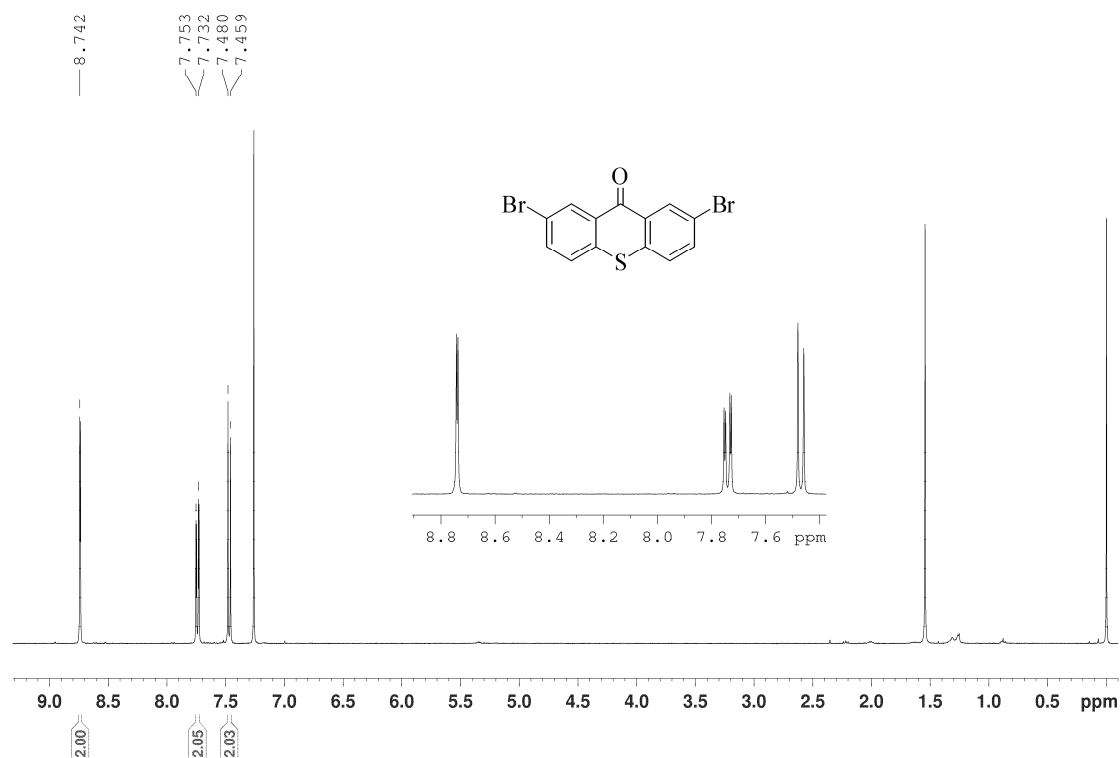


Figure S1. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **DB-TXO**.

Monoisotopic Mass, Odd and Even Electron Ions
15 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-15 H: 0-10 O: 0-1 S: 0-2 Br: 0-2

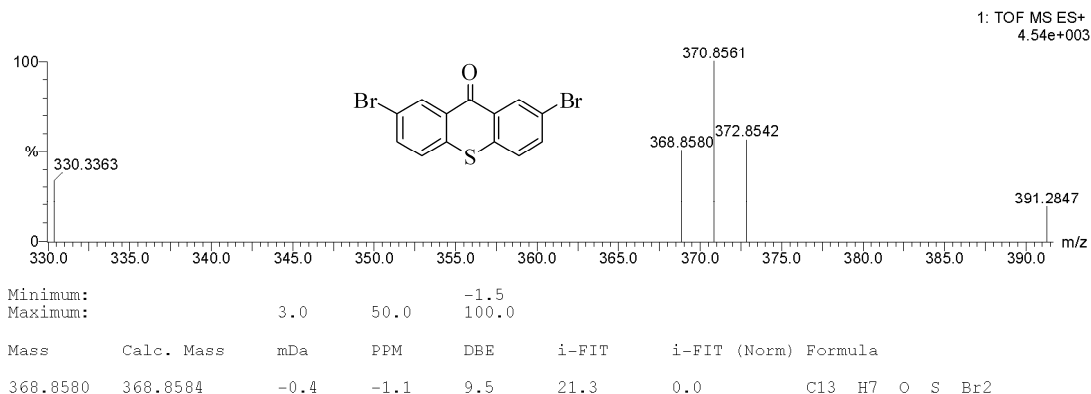


Figure S2. ESI-MS spectrum of compound **DB-TXO**.

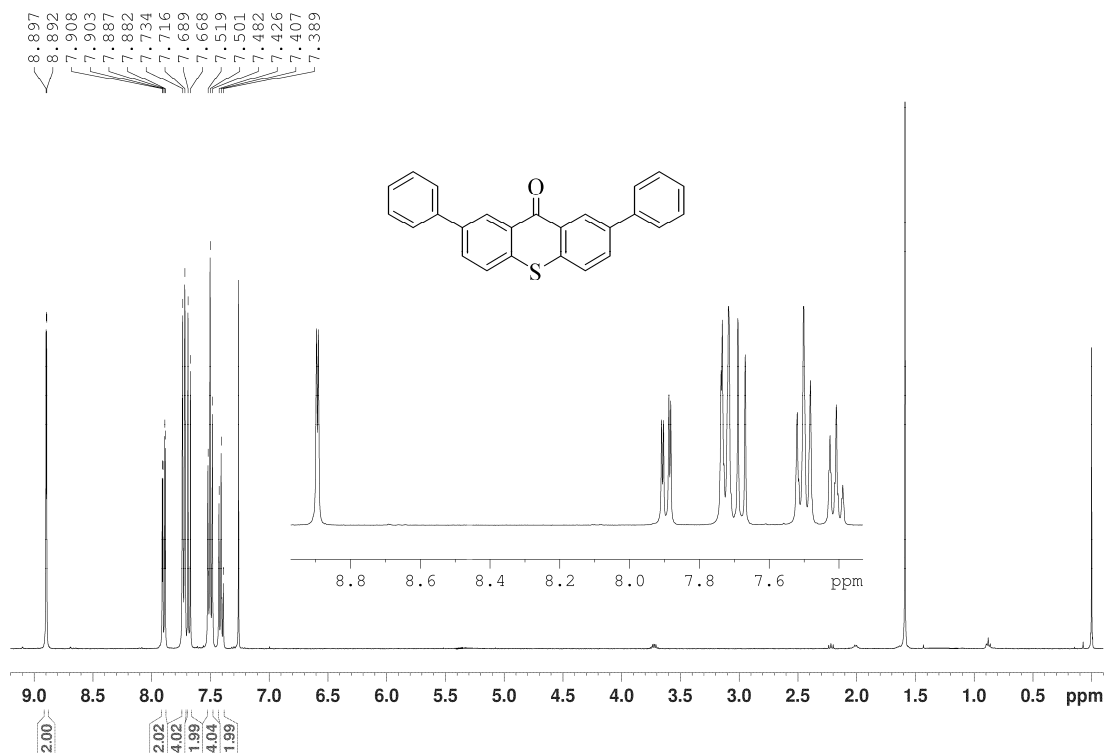


Figure S3. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **DP-TXO**.

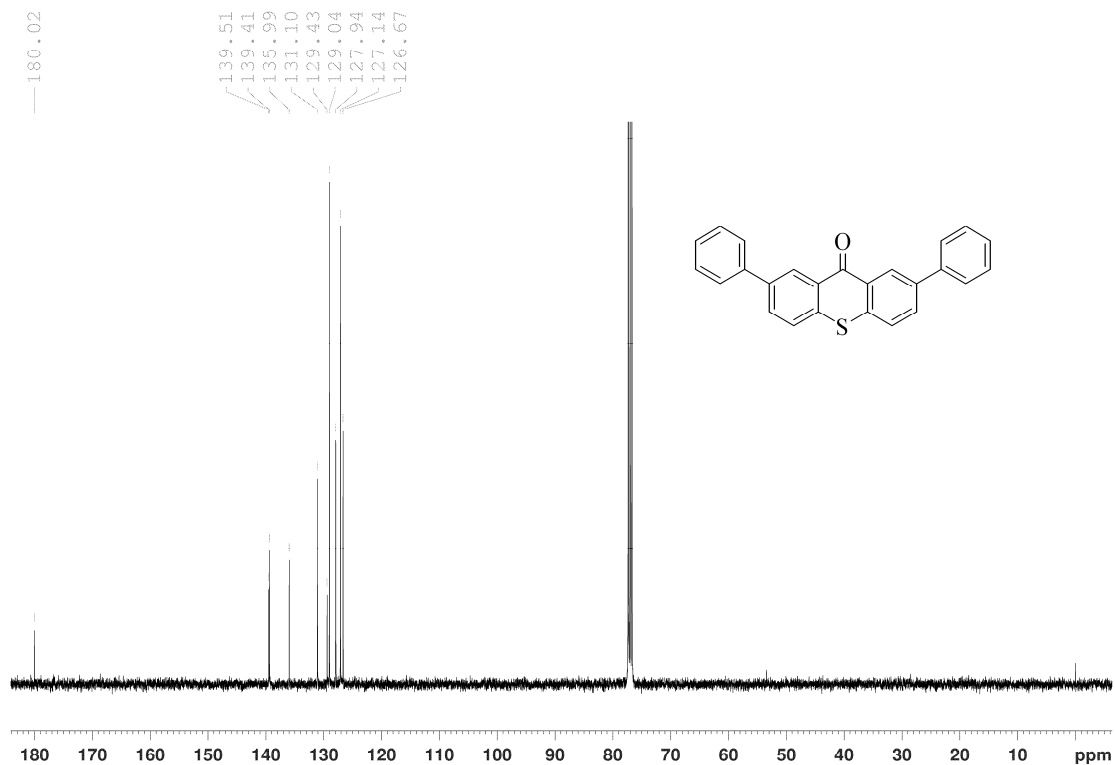


Figure S4. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound **DP-TXO**.

Monoisotopic Mass, Even Electron Ions

217 formula(e) evaluated with 188 results within limits (up to 1 closest results for each mass)

Elements Used:

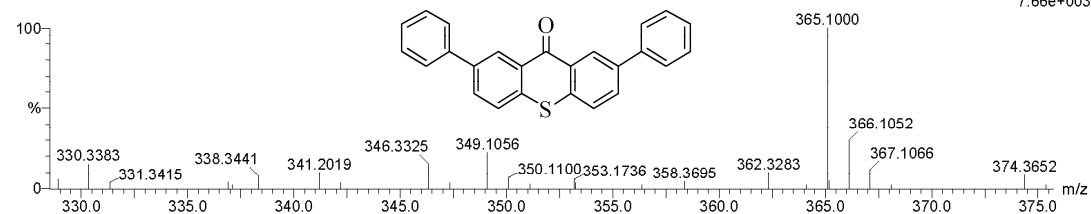
C: 0-80 H: 0-160 O: 0-16 S: 0-3

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20-Oct-2011

19:56:46

1: TOF MS ES+
7.66e+003



Minimum:

Maximum: 500.0 50.0 -1.5 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
365.1000	365.1000	0.0	0.0	17.5	21.4	0.0	C ₂₅ H ₁₇ O S

Figure S5. ESI-MS spectrum of compound **DP-TXO**.

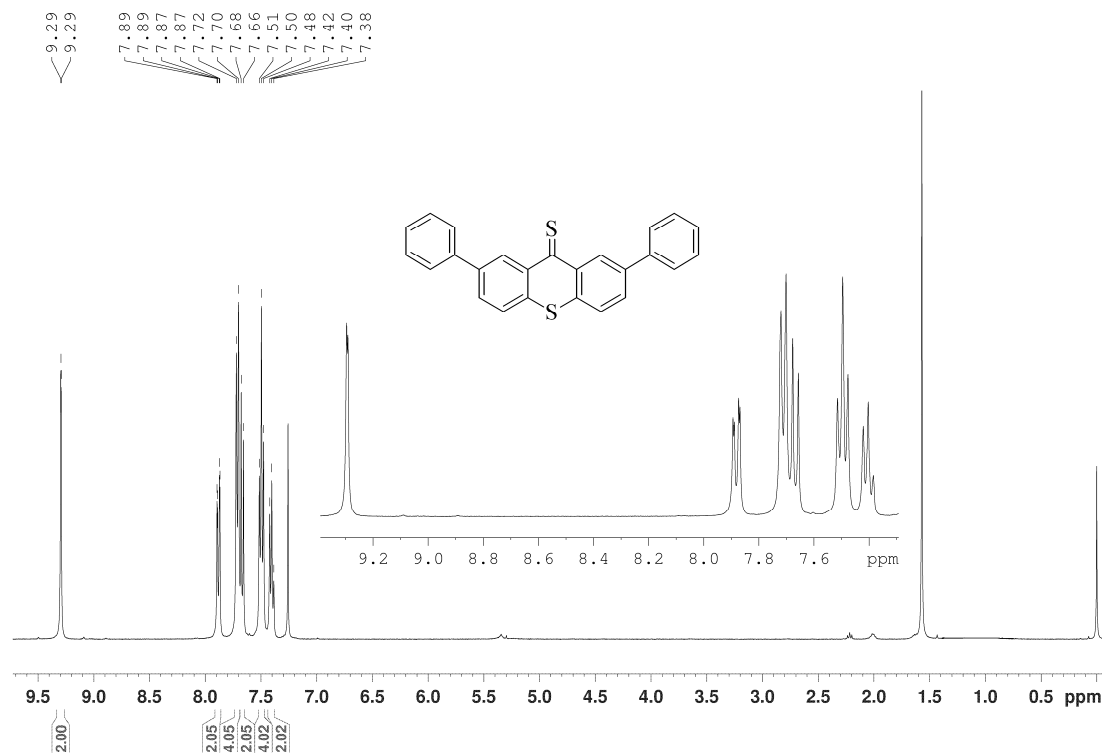


Figure S6. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **DP-TXT**.

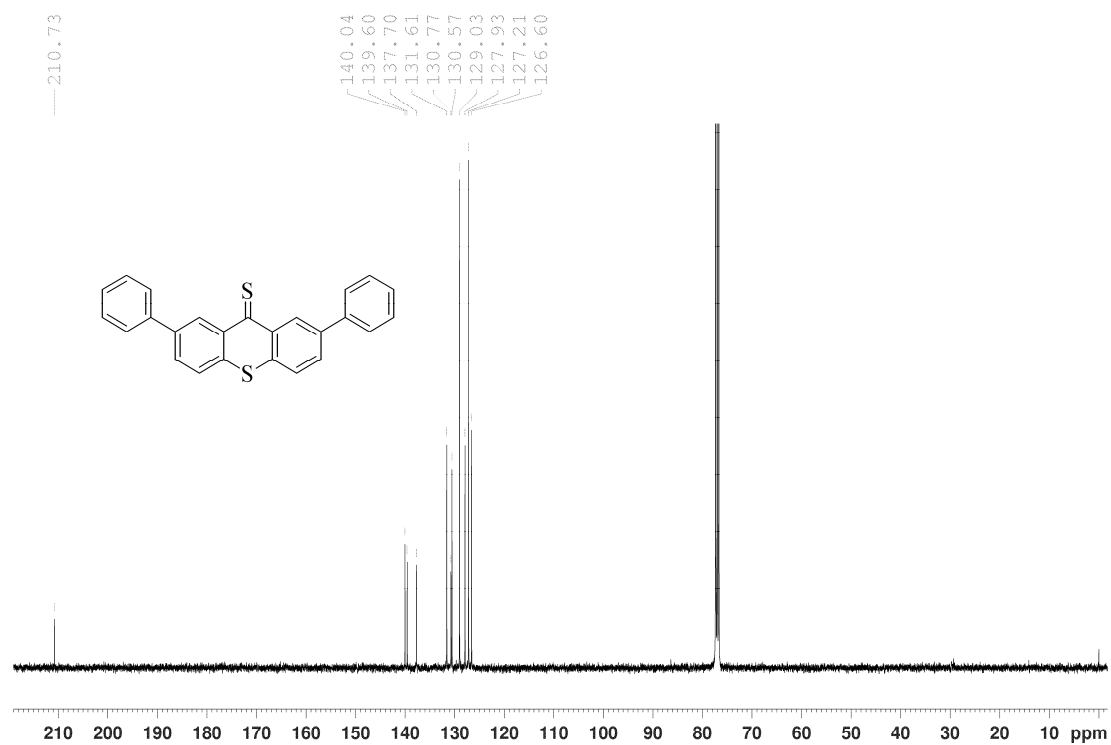


Figure S7. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound **DP-TXT**.

Monoisotopic Mass, Even Electron Ions

2 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 0-25 H: 0-20 S: 0-2

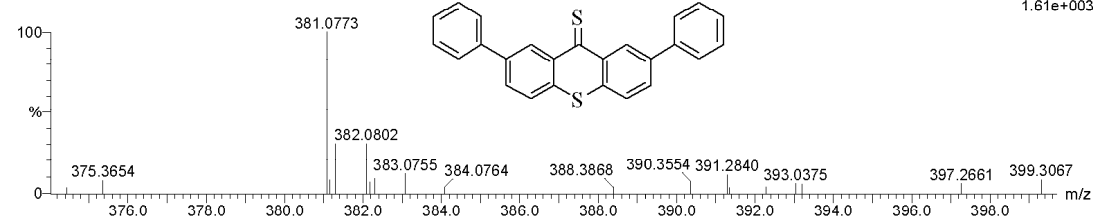
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26-Oct-2011

21:57:55

1: TOF MS ES+

1.61e+003



Minimum:				-1.5			
Maximum:	50.0	50.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
381.0773	381.0772	0.1	0.3	17.5	47.6	0.0	C25 H17 S2

Figure S8. ESI-MS spectrum of compound **DP-TXT**.

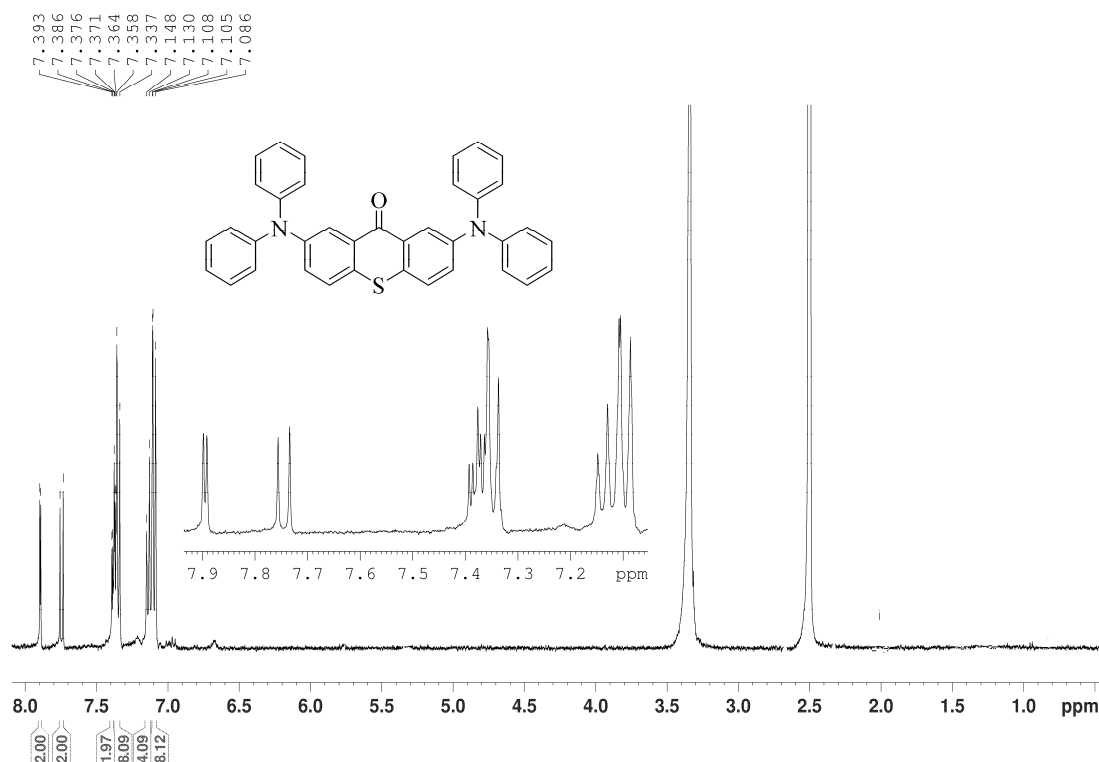


Figure S9. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of compound **BDPA-TXO**.

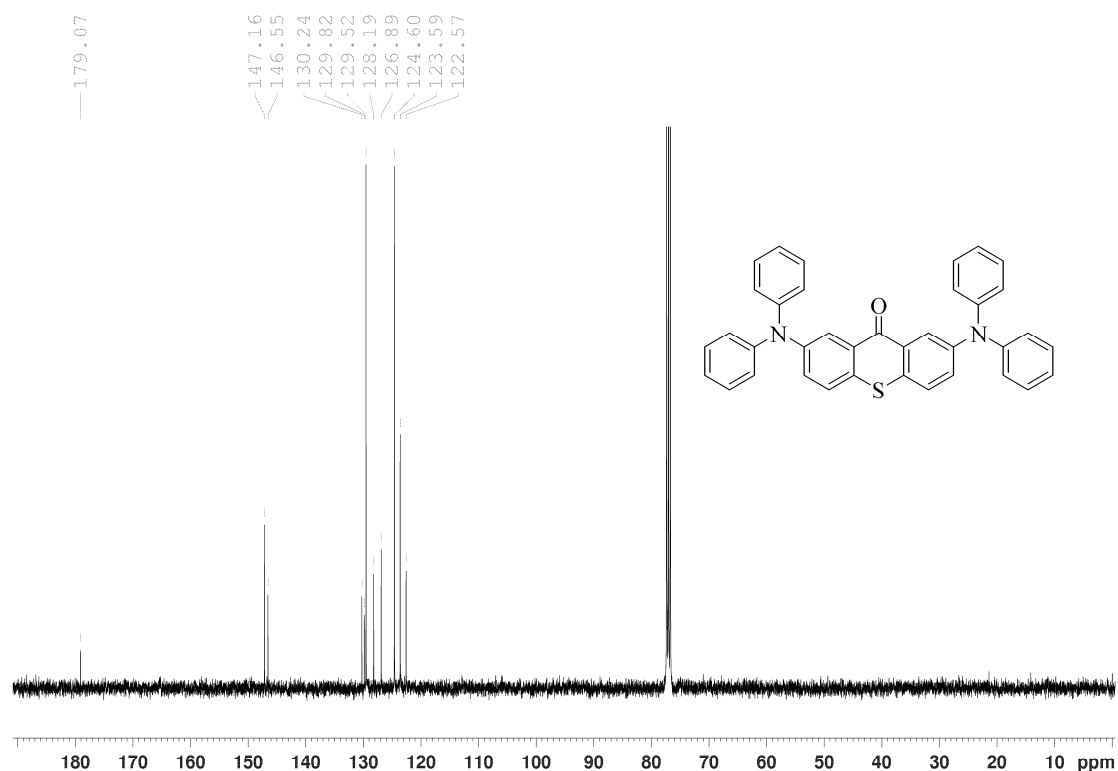


Figure S10. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **BDPA-TXO**.

Monoisotopic Mass, Even Electron Ions

72 formula(e) evaluated with 8 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 0-40 H: 0-30 N: 0-5 O: 0-1 S: 0-2

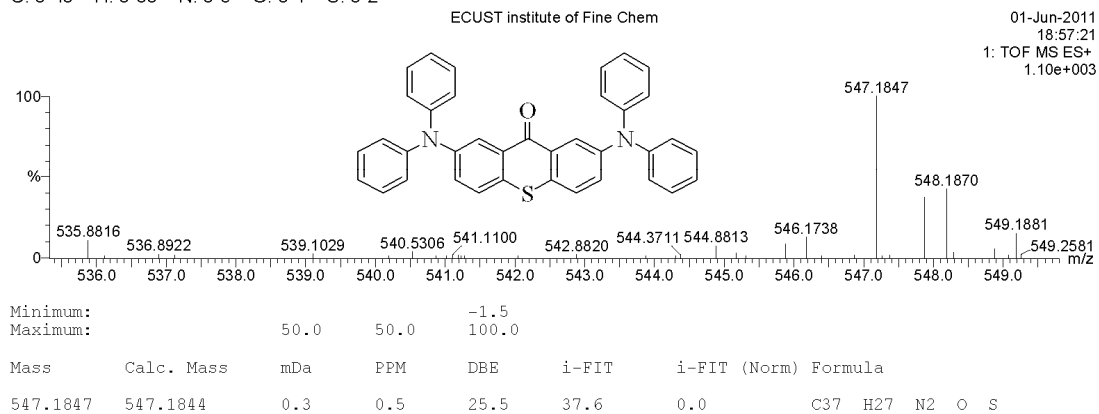


Figure S11. ESI-MS spectrum of compound **BDPA-TXO**.

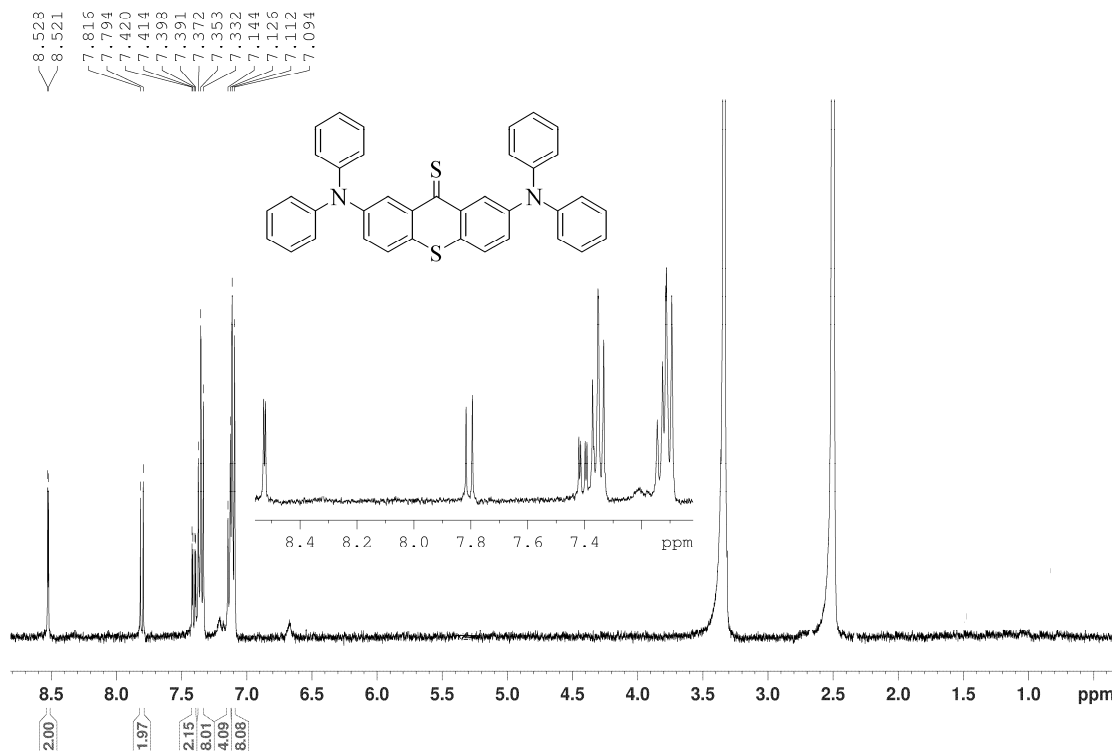


Figure S12. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of compound **BDPA-TXT**.

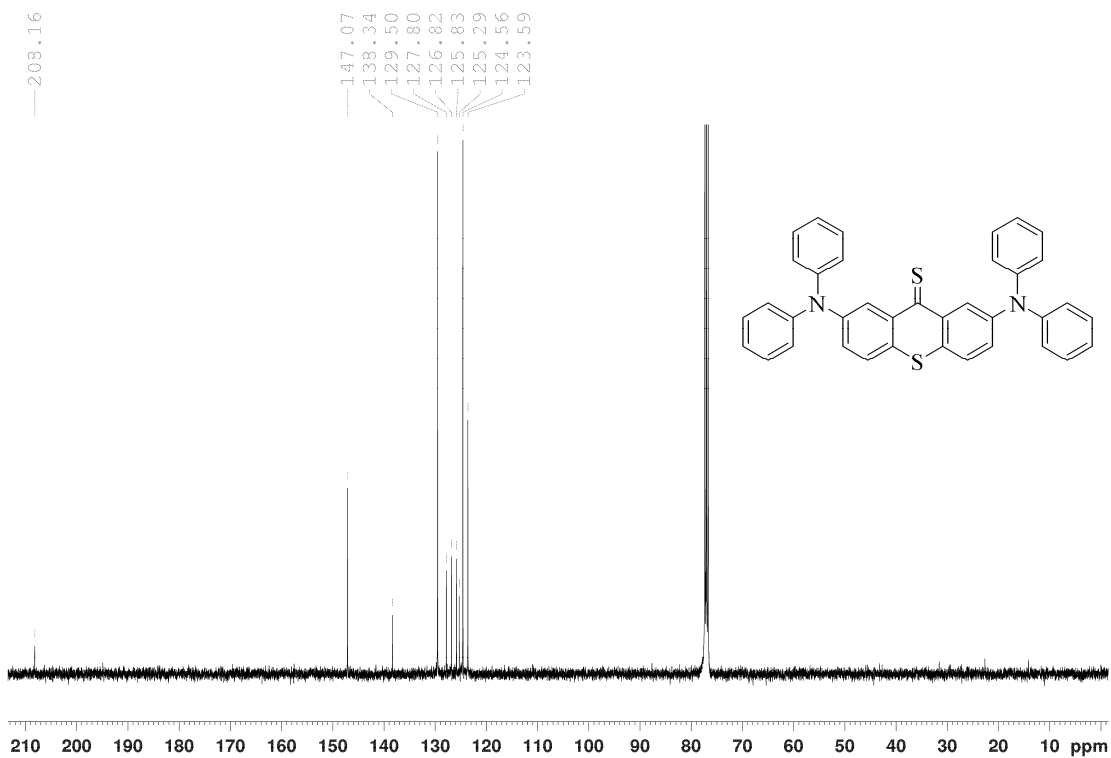


Figure S13. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **BDPA-TXT**.

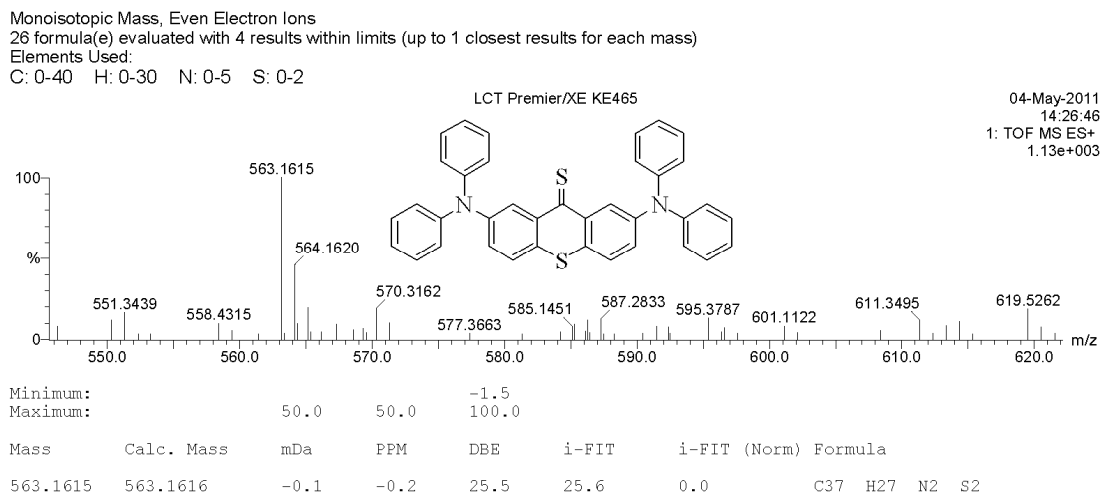


Figure S14. ESI-MS spectrum of compound **BDPA-TXT**.

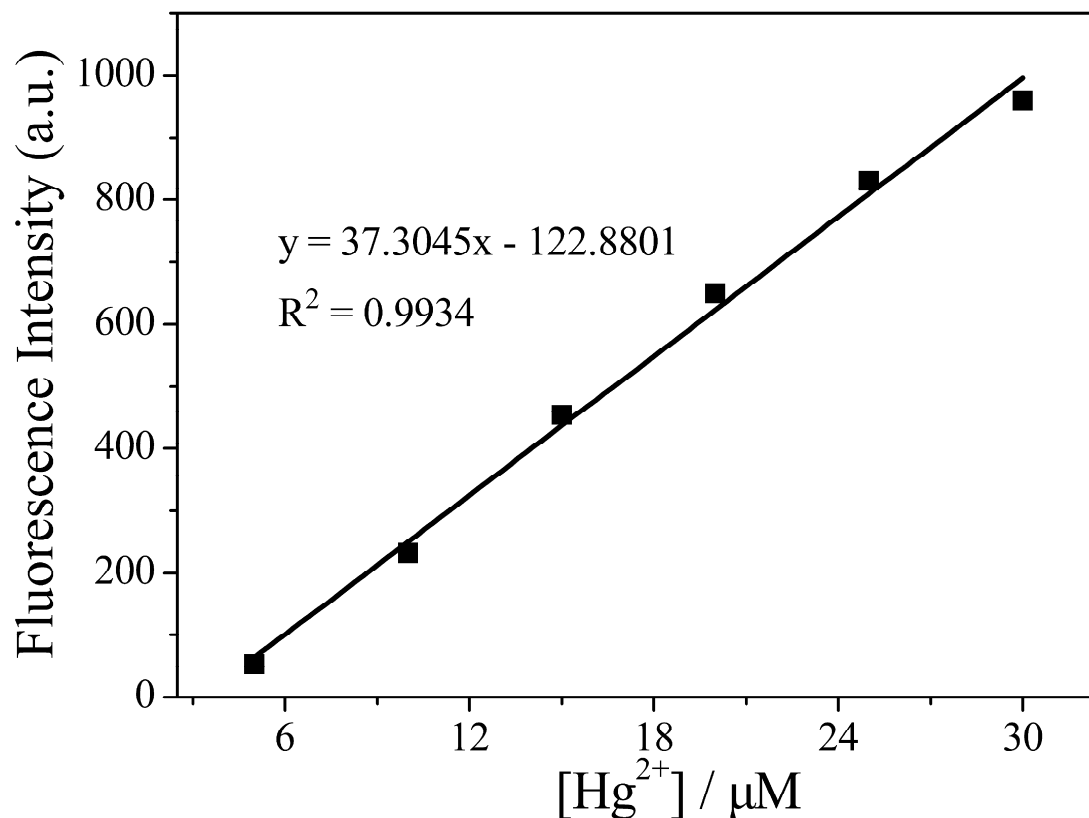


Figure S15. A plot of fluorescence intensity change of **DP-TXT** (10.0 μM) against varied concentrations of Hg^{2+} (5.0–30.0 μM) in $\text{CH}_3\text{CN}-\text{H}_2\text{O}$ (5:5, v/v) ($\lambda_{\text{ex}} = 309 \text{ nm}$, slit: 5 nm/5 nm, PMT Volts: 610.). $R^2 = 0.9934$, $k = 3.7 \times 10^7 \text{ au/M}$. The Standard deviation ($\sigma = 0.26$) 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 ($3\sigma/k$) and gave a result 21 nM.

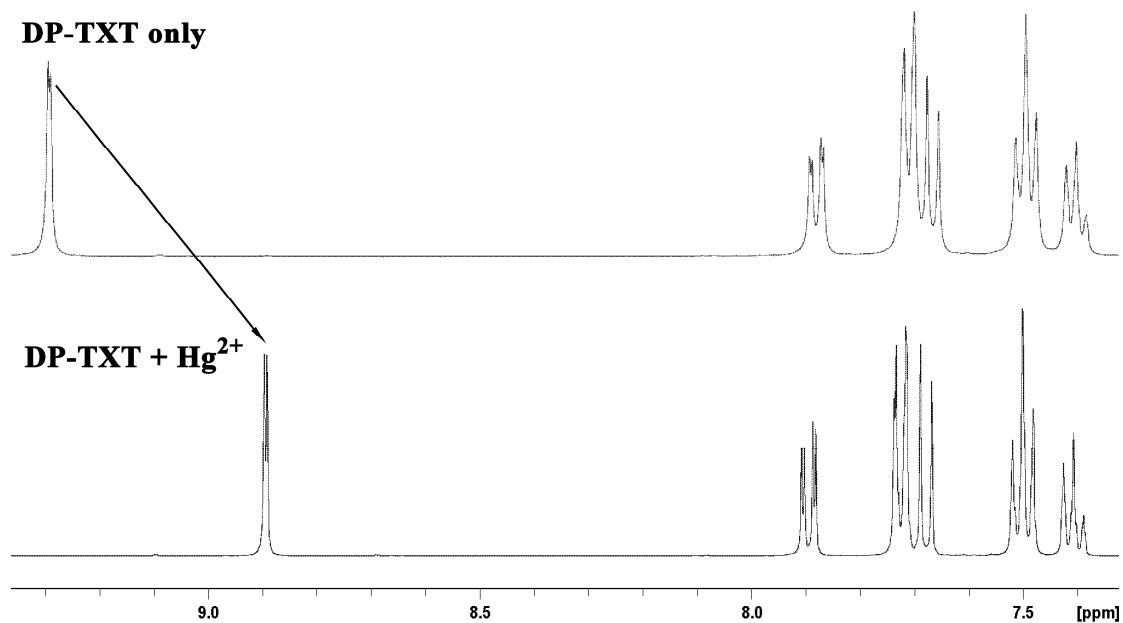


Figure S16. Partial ¹H NMR spectrum (400 MHz, CDCl₃) of chemodosimeter DP-TXT before and after addition of excessive Hg²⁺

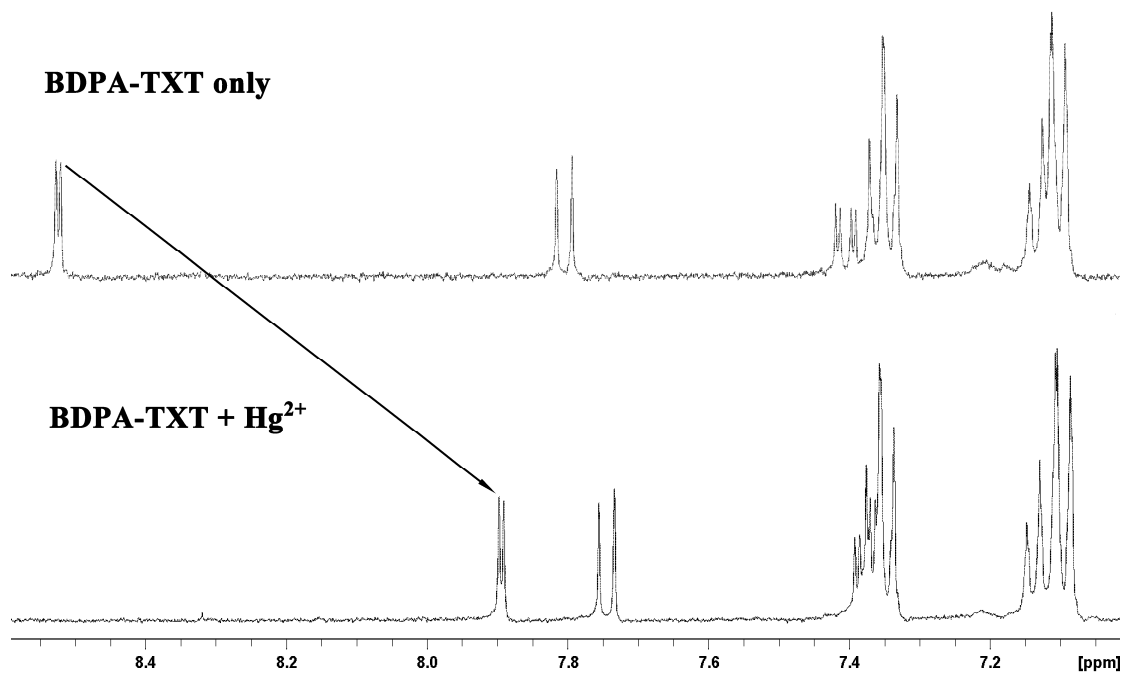


Figure S17. Partial ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of chemodosimeter BDPA-TXT before and after addition of excessive Hg²⁺

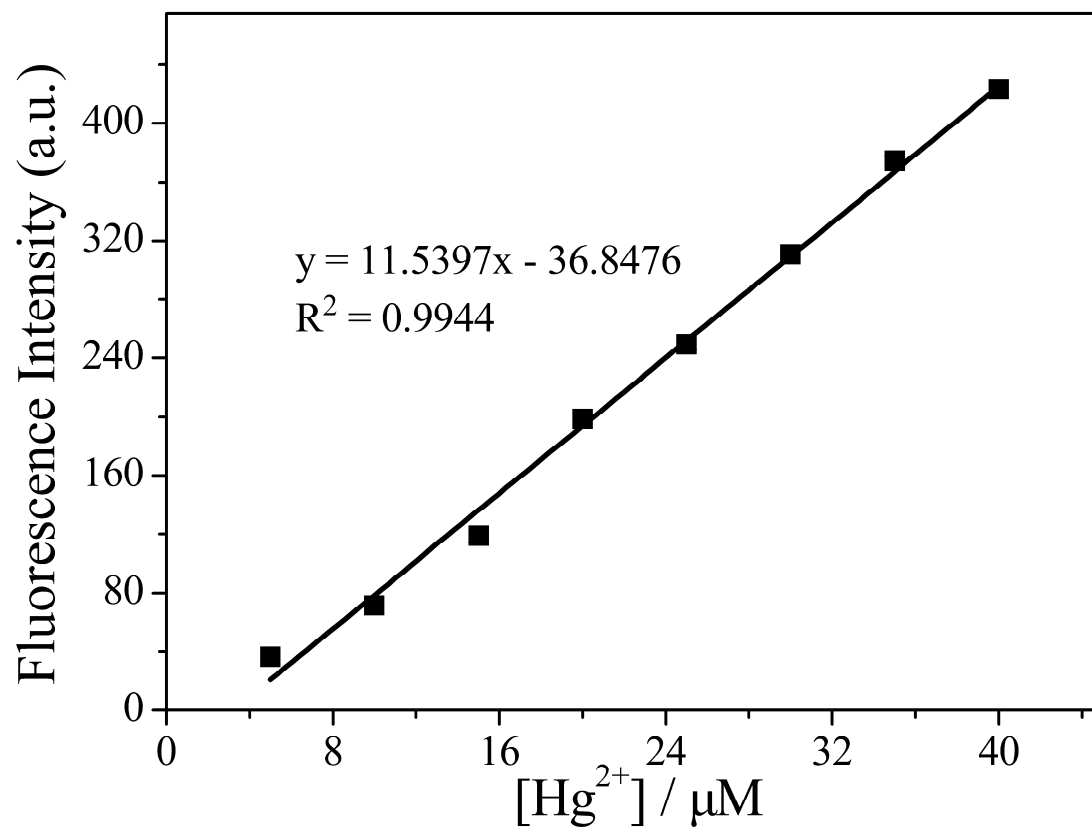
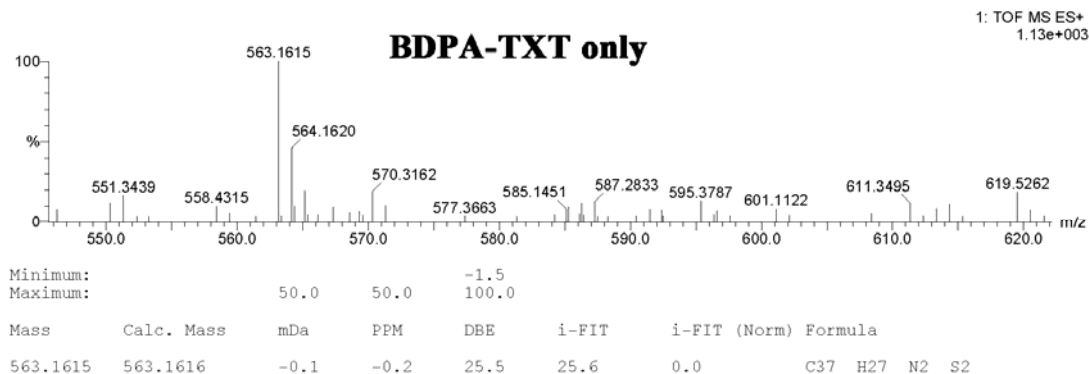


Figure S18. A plot of fluorescence intensity change of **BDPA-TXT** (10.0 μM) against varied concentrations of Hg^{2+} (5.0–40.0 μM) in DMSO–H₂O (9:1, v/v) ($\lambda_{\text{ex}} = 357$ nm, slit: 5 nm/5 nm, PMT Volts: 800.). $R^2 = 0.9944$, $k = 1.2 \times 10^7$ au/M. The Standard deviation ($\sigma = 0.30$) 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 ($3\sigma/k$) and gave a result 75 nM.

Monoisotopic Mass, Even Electron Ions
26 formula(e) evaluated with 4 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-40 H: 0-30 N: 0-5 S: 0-2



Monoisotopic Mass, Even Electron Ions
72 formula(e) evaluated with 8 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-40 H: 0-30 N: 0-5 O: 0-1 S: 0-2

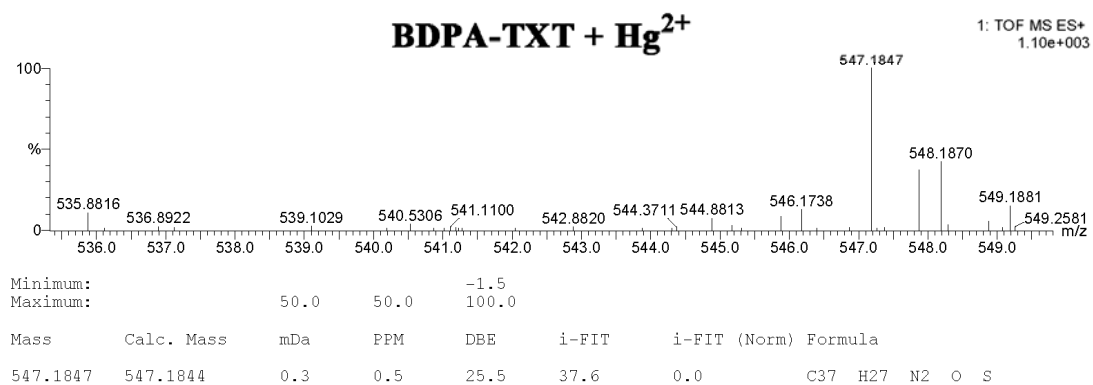
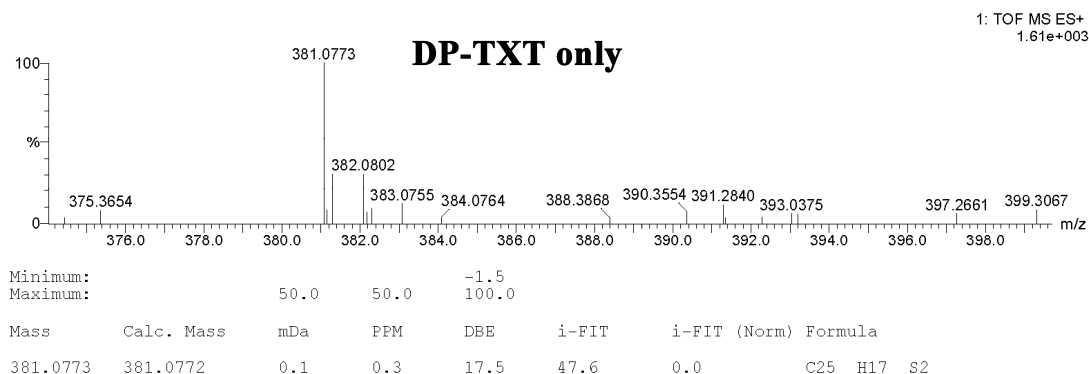


Figure S19. HRMS (ESI) spectra of compound **BDPA-TXT** in the absence and in the presence of Hg²⁺.

Monoisotopic Mass, Even Electron Ions
 2 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
 Elements Used:
 C: 0-25 H: 0-20 S: 0-2



Monoisotopic Mass, Even Electron Ions
 217 formula(e) 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

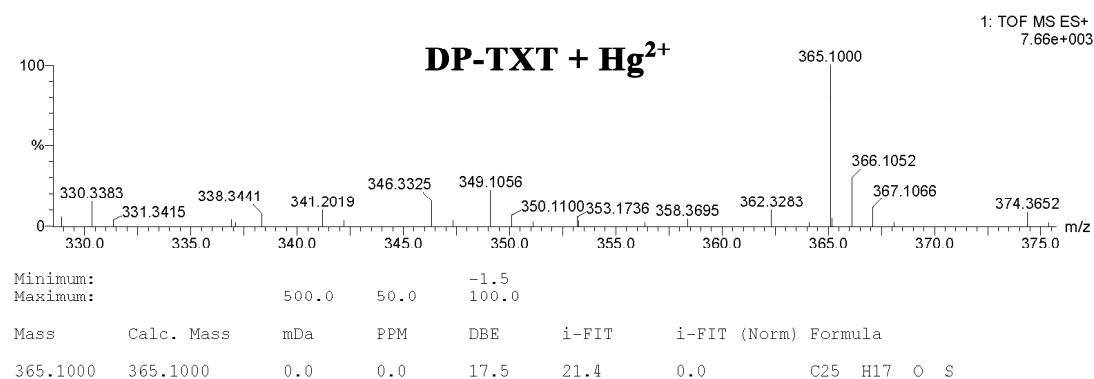


Figure S20. HRMS (ESI) spectra of compound **DP-TXT** in the absence and in the presence of Hg²⁺.

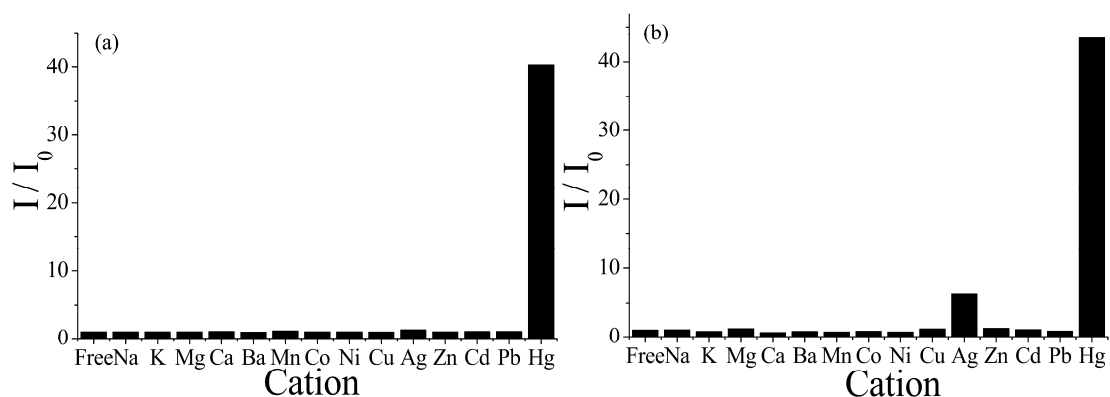


Figure S21. (a) Emission ratiometric response of **DP-TXT** to various metal ions. [DP-TXT] = 1.0×10^{-5} M, [Hg²⁺] = 3.0×10^{-5} M, [Mⁿ⁺] = 1.0×10^{-4} M. (b) Emission ratiometric response of **BDPA-TXT** to various metal ions. [BDPA-TXT] = 1.0×10^{-5} M, [Hg²⁺] = 4.0×10^{-5} M, [Mⁿ⁺] = 1.0×10^{-4} M.