

Supplementary information

for

A Fluorometric/Colorimetric Dual-channel Hg²⁺ Sensor Derived from 4-Amino-7-nitro-benzoxadiazole (ANBD) Fluorophore

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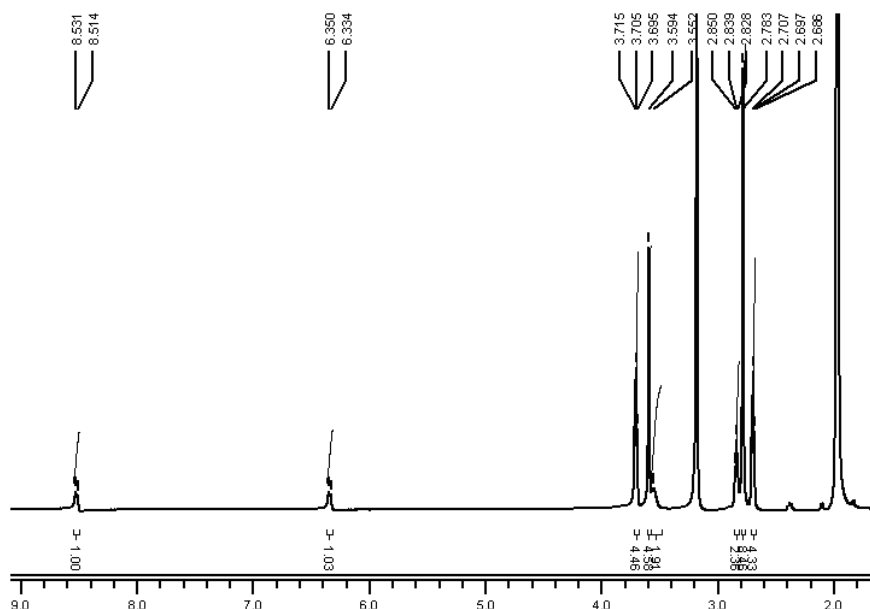


Figure S1. ¹H NMR spectrum of NBD-TAEE in CD₃CN.

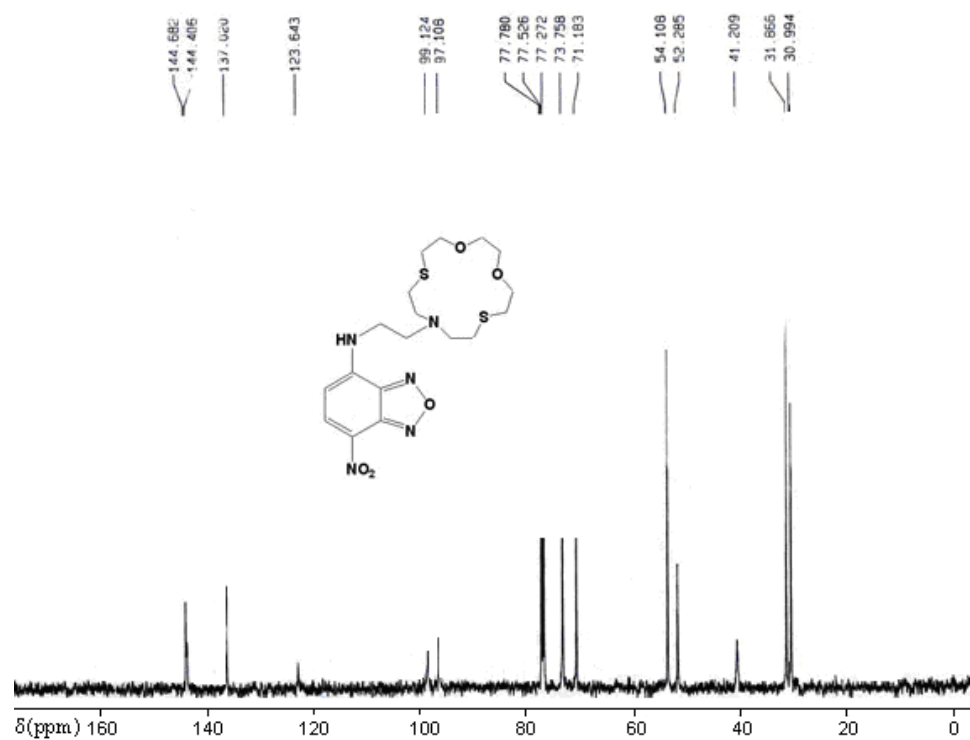


Figure S2. ^{13}C NMR spectrum of NBD-TAEE in CDCl_3 .

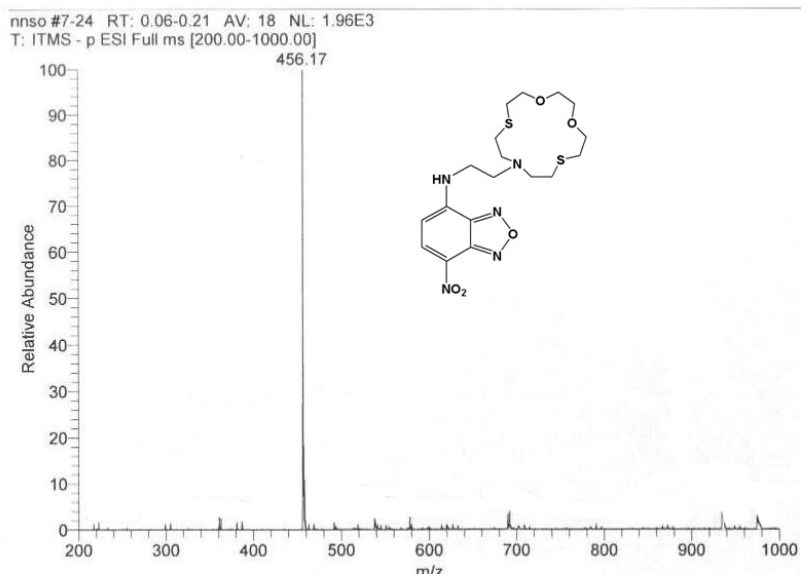


Figure S3. ESI-MS spectrum of NBD-TAEE.

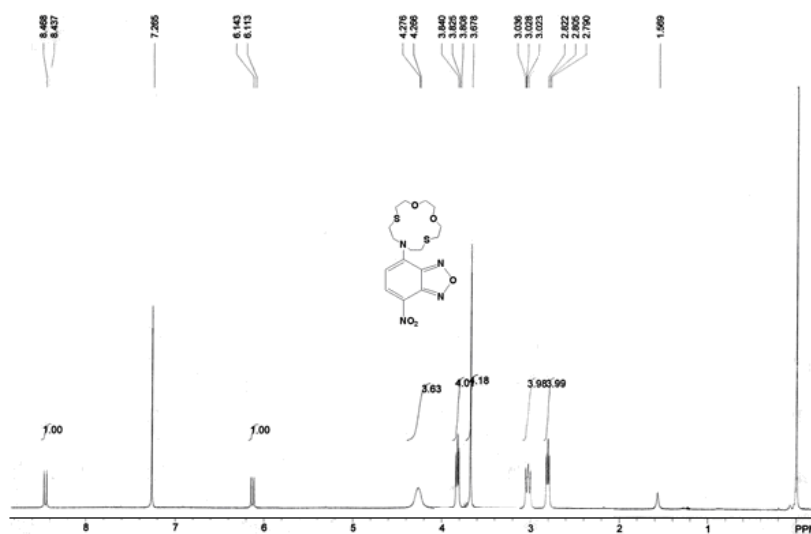


Figure S4. ^1H NMR spectrum of NBD-TAE in CDCl_3 .

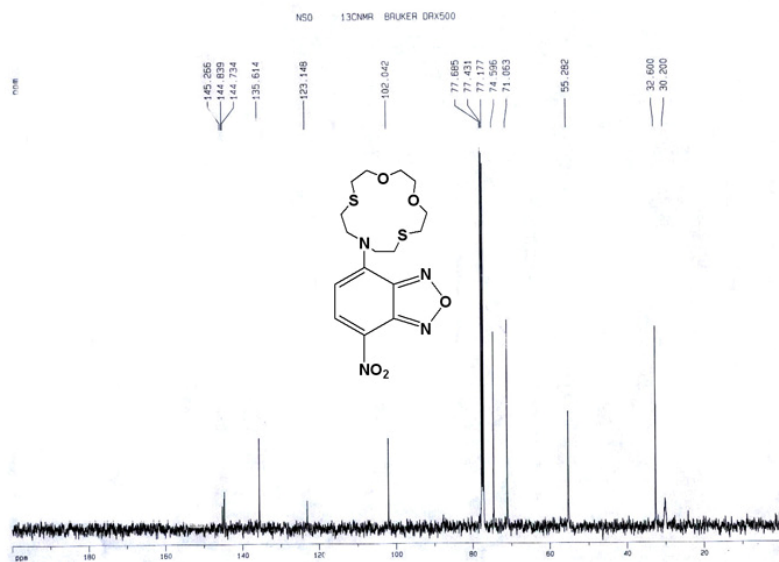


Figure S5. ^{13}C NMR spectrum of NBD-TAE in CDCl_3 .

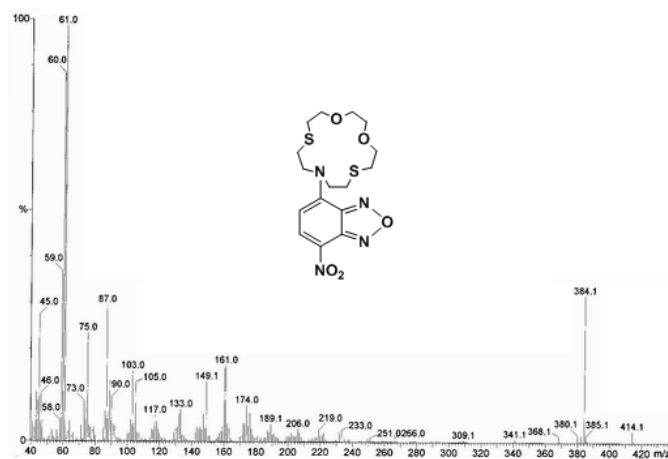


Figure S6. MS spectrum (EI) of NBD-TAE.

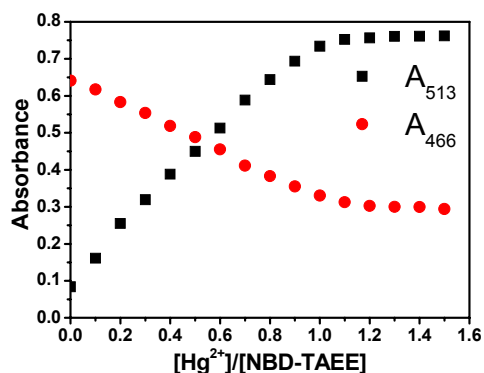


Figure S7. UV-vis titration profiles of NBD-TAEE (25 μM) in acetonitrile containing 5% (v/v) HEPES buffer (20 mM; 50 mM KNO_3 ; pH 7.2) according to the absorbance at 513 and 466 nm.

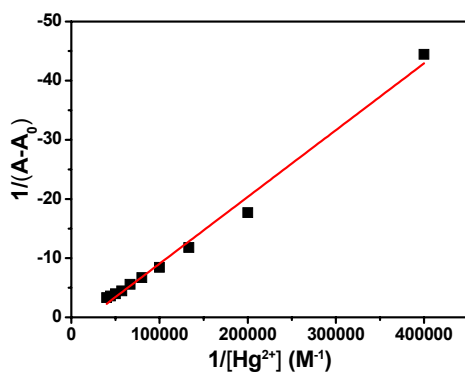


Figure S8. Plot of $1/\Delta A_{466}$ against $1/[M]$ based on the UV-vis Hg^{2+} titration of NBD-TAEE (■). Data are based on the absorbance at 466 nm. The line represents the fitting result via Benesi-Hilderbrand fitting. ($R = 0.995$).

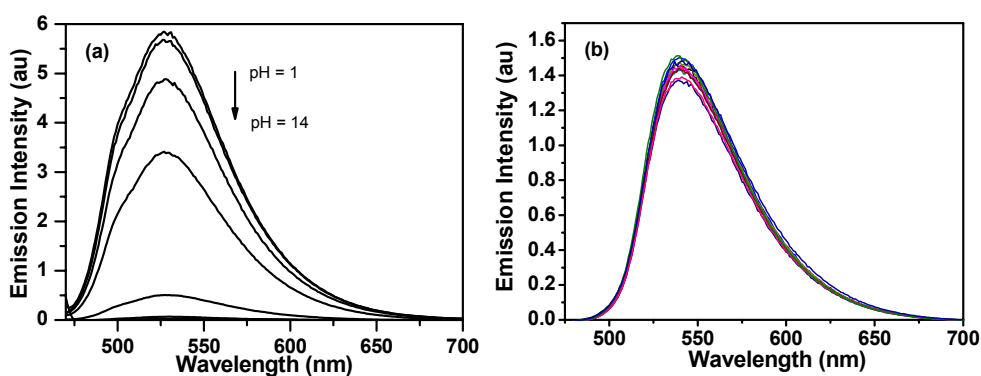


Figure S9. Emission spectra of NBD-TAEE (a) and NBD-TAE (b) in aqueous acetonitrile (acetonitrile/water: 95/5, v/v) at different pH.

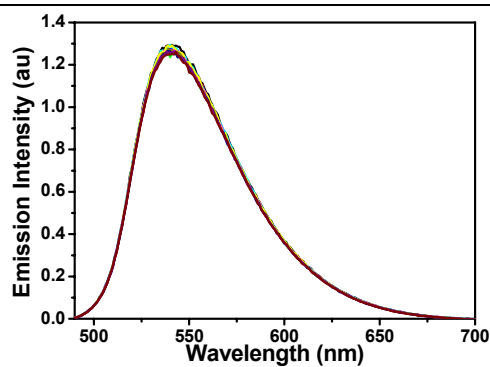


Figure S10. Emission spectra of **NBD-TAE** (25 μM) in acetonitrile containing 5% (v/v) HEPES buffer (20 mM; 50 mM KNO_3 ; pH 7.2) in the presence of different $[\text{Hg}^{2+}]_{\text{total}}$. λ_{ex} , 466 nm. The $[\text{Hg}^{2+}]_{\text{total}}$ varies from 0 to 125 μM .

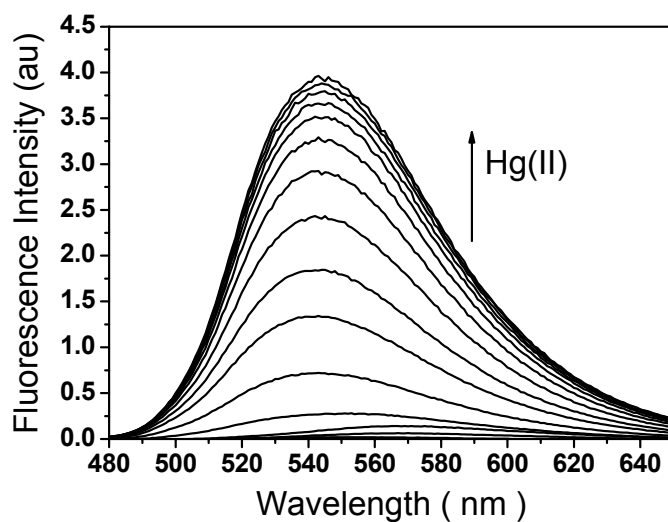


Figure S11. Emission spectra of **NBD-TAEE** (25 μM) in DMSO in the presence of different $[\text{Hg}^{2+}]_{\text{total}}$. $[\text{Hg}^{2+}]_{\text{total}}$ increase from 0 to 32.5 μM along the arrow.

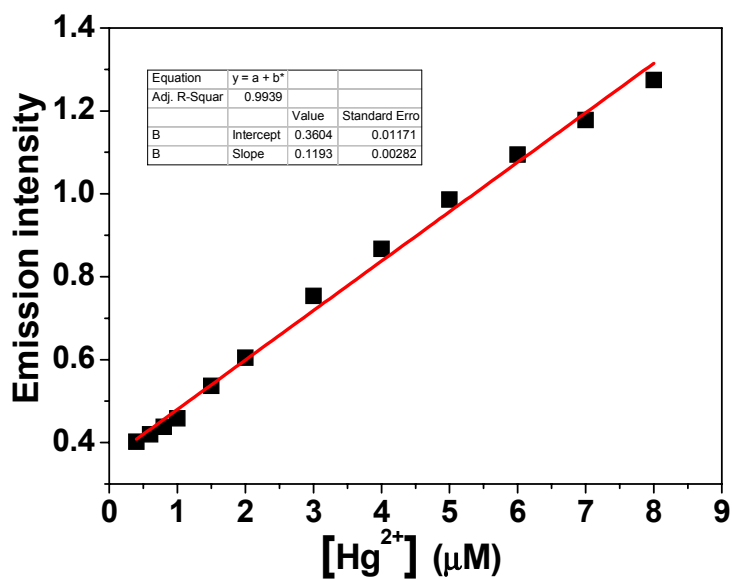


Figure S12. The fluorescent response of **NBD-TAEE** (10 μM) in acetonitrile containing 5% (v/v) HEPES buffer (20 mM; 50 mM KNO₃; pH 7.2) upon the addition of Hg²⁺.